IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant: Jonathan Scott Brecher

Serial No.:   To Be Assigned

Filed: Herewith (This application claims the benefit of U.S. Provisional Application Serial No.
               60/119,930 entitled DERIVING A CHEMICAL STRUCTURE FROM A
               CHEMICAL NAME, filed on February 12, 1999.)

Title: DERIVING CHEMICAL STRUCTURAL INFORMATION

Box Patent Application
Assistant Commissioner for Patents
Washington, DC 20231

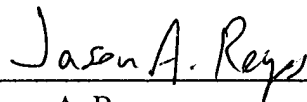## COVER SHEET FOR APPENDIX: NOMTOKENS

Dear Sir:

    Enclosed for filing in the above-referenced patent application is the following document:

1.   Appendix: NOMTOKENS, 111 pages.

The following is the inventor's residence:
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                                 Respectfully submitted,

Dated: February 11, 2000

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                              EXPRESS MAIL LABEL NO. EM259723548US

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meth|carbin root alkane C,a|alpha|1|w|omega
carbenium root root [C+],1|w|omega
carbene root root C,32@1|w|omega
aminylene|nitrene root root N,32@1|w|omega
hydroxymethyl root root C,4@x,O,x
hydroxymethylene root root C,8@x,O,x
form root trivial C,x|1|w|omega,(=O),x
formimino root trivial C,4@x|1|w|omega,(=N),x
formalin root root C=O,x
eth root alkane C,1|a|alpha,C,2|b|beta|w|omega
ethene|ethen root alkane C,1|a|alpha,=,x,C,2|b|beta|w|omega
ethyne|ethyn root alkane C,1|a|alpha,#,x,C,2|b|beta|w|omega
acet root trivial C,1,(=,x,O,x,),x,C,2|a|alpha|w|omega
aceto root trivial C,4@1,(=,x,O,x,),x,C,2|a|alpha|w|omega
acetoacet|acetoaceto root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3,(=,x,O,x,),x,C,4|g|gamma|w|omega
prop|propa root alkane C,1|a|alpha,C,2|b|beta,C,3|g|gamma|w|omega
isoprop|isopropa|isopropion root alkane C,a|alpha,(,x,C,b|beta,),x,C,x
hexafluoroisoprop|hexafluoroisopropa root alkane
C,a|alpha,(C(F)(F)F),x,C(F)(F)F,x
propiono|propion|propio|propi root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta|w|omega
proparg|proparag root alkane C,1|a|alpha,C,2,#,x,C,3|w|omega
tetrol loveracid alkane C,1,C,2,#,x,C,3,C,4|w|omega
but|buta root alkane C,1|a|alpha,C,2|b|beta,C,3|g|gamma,C,4|d|delta|w|omega
butyro|butyr root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma|w|omega
isobutyro|isobutyr root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(,x,C,3|b|beta,),x,C,4|b'|beta'|g|gamma|w|omega
isobutylene root root C=C(C)C,x
crotono|croton root trivial
C,1,(=,x,O,x,),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
crot root root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
crotonylalcohol root root
C,1,(O),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
isocrotono|isocroton root trivial
C,1,(=,x,O,x,),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
isocrot root root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
seneci root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,=,x,C,3|b|beta,(,x,C,4|g|gamma|w|omega,),x,C,4'|g'|
gamma'|w'|omega'
tigl|cevad root trivial
C,1,(=,x,O,x,),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
angel root trivial
C,1,(=,x,O,x,),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
pren root alkane C,1,C,2|a|alpha,=,x,C,3|b|beta,(C),x,C,4|g|gamma|w|omega
valero|valer|valerian root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
acetonoxal root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(=O),x,C,3|b|beta,C,4|g|gamma,(=O),x,C,5|d|delta|w|
omega
valpr root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(CCC),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
levulin|laevulin|levul root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4,(=O),x,C,5|g|gamma|d|delta|w|omega
isovalero|isovaler|delphin root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,(,x,C,4|g|gamma,),x,C,5|d|delta|w|omega

pival root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(,x,C,3|b|beta,)(,x,C,4|3',),x,C,5|3''
amyl root alkane C,4@1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
capro root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon|w|omega
acexam root root
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,N,x,C,x,(=O),x,
C,x,
enatho|enanth|oenantho|oenanth root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7|w|omega
geron root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(C)(C),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|e
psilon,(=O),x,C,7|w|omega
capryl root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8|w|omega
octoate root root
O,1@x,C,1,(=O),x,C,2|a|alpha,(,x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilo
n,),x,C,x,C,x
pelargono|pelargon|pelarg|pergon root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9|w|o
mega
capr root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0|w|omega
obtusil root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
,C,10|w|omega
stilling root alkane
C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma,=,x,C,5|d|delta,\,x,C,6|e|eps
ilon,C,7,C,8,C,9,C,10|w|omega
lauro|laur|vulv|laurostear root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12|w|omega
linder root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
,C,10,C,11,C,12|w|omega
myristo|myrist root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14|w|omega
physeter|physoter root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,=,x,C,6|e|epsilon,C,7,C,8,C,9
,C,10,C,11,C,12,C,13,C,14|w|omega
ipurol root alkane
C,1,C,2|a|alpha,C,3|b|beta,(O),x,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
,9,C,10,C,11,(O),x,C,12,C,13,C,14|w|omega
tsuzu|tudu root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
,C,10,C,11,C,12,C,13,C,14|w|omega
myristelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,/,x,C,11,C,12,C,13,C,14|w|omega
myristole root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,\,x,C,11,C,12,C,13,C,14|w|omega
palmito|palmit|cet root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16|w|omega

palmitelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
palmitole root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
hiragon root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,=,x,C,7,C,8,C,9
,C,10,=,x,C,11,C,12,C,13,C,14,=,x,C,15,C,16|w|omega
ustil root alkane
C,1,C,2|a|alpha,(O),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
,9,C,10,C,11,C,12,C,13,C,14,C,15,(O),x,C,16|w|omega,O,x
ambrettol root alkane
C,1,C,2|a|alpha,(O),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,=,x,C
,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,O,x
aleurit root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(O)
,x,C,10,(O),x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,O,x
gaid|hypogae root alkane
C,1,C,2|a|alpha,=,x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
juniper root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,O,x
margaro|margar root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17|w|omega
stear|stearophan root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
moroct root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,=,x
,C,9,C,10,C,11,C,12,=,x,C,13,C,14,C,15,=,x,C,16,C,17,C,18|w|omega
parinar root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,=,x
,C,10,C,11,=,x,C,12,C,13,=,x,C,14,C,15,=,x,C,16,C,17,C,18|w|omega
eleostear root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,\,x,C,11,=,x,C,12,/,x,C,13,=,x,C,14,\,x,C,15,C,16,C,17,C,18|w|omega
stearol loveracid root
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,#,x
,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
couep|lican root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,(=O),x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,
C,9,=,x,C,10,C,11,=,x,C,12,C,13,=,x,C,14,C,15,C,16,C,17,C,18|w|omega
trichosan root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,/,x,C,11,=,x,C,12,\,x,C,13,=,x,C,14,/,x,C,15,C,16,C,17,C,18|w|omega
floionol|phloionol root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(O)
,x,C,10,(O),x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega,O,x
lycaon root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,(=O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
lactarin root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,(=O),x,C,7,C,8,
C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

jalapinol root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,(O),x,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
ole root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
elaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
ricinole|ricinol root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,\,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
ricinelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,/,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
linole|telfair root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,\,x,C,11,/,x,C,12,=,x,C,13,\,x,C,14,C,15,C,16,C,17,C,18|w|omega
vernol loveracid root CCCCCCCC\C=C/C[C@H]1[C@@H](CCCCC)O1,x
linolelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,/,x,C,11,/,x,C,12,=,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega
linolenelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,/,x,C,11,/,x,C,12,=,x,C,13,/,x,C,14,/,x,C,15,=,x,C,16,/,x,C,17,C,18|w|
omega
linolen|alphalinolen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,\,x,C,11,/,x,C,12,=,x,C,13,\,x,C,14,/,x,C,15,=,x,C,16,\,x,C,17,C,18|w|
omega
gammalinolen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,=,x,C,7,\,x
,C,8,/,x,C,9,=,x,C,10,\,x,C,11,/,x,C,12,=,x,C,13,\,x,C,14,C,15,C,16,C,17,C,18|w|
omega
vaccen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,/,x,C,11,=,x,C,12,/,x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
petroselaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,=,x,C,7,/,x
,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
petroselin root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,=,x,C,7,\,x
,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
calend root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,/,x,C,8,=,x
,C,9,\,x,C,10,=,x,C,11,\,x,C,12,=,x,C,13,\,x,C,14,C,15,C,16,C,17,C,18|w|omega
arachido|arachid|arachin root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega
gadole root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega
arachidon root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,/,x,C,5|d|delta,=,x,C,6|e|epsilon,\,x,C,7
,/,x,C,8,=,x,C,9,\,x,C,10,/,x,C,11,=,x,C,12,\,x,C,13,/,x,C,14,=,x,C,15,\,x,C,16,
C,17,C,18,C,19,C,20|w|omega

arach root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21|w|omega
lesquerol root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,/,x,C,11,=,x,C,12,\,x,C,13,[C@H],14,(O),x,C,15,C,16,C,17,C,18,C,19,C,20,C,21|w
|omega
beheno|behen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22|w|omega
eruc root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,/,x,C,13,=,x,C,14,\,x,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22|w|omeg
a
brassid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,/,x,C,13,=,x,C,14,/,x,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22|w|omeg
a
lignocero|lignocer root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24|w|omega
cerebron|phrenosin root alkane
C,1,C,2|a|alpha,(O),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24|w|
omega
nervon root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,/,x,C,15,=,x,C,16,\,x,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C
,24|w|omega
hyen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25|w|o
mega
cerotino|cerotin|cerot|cerane root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
6|w|omega
ceryl root alkane
C,4@1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C
,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C
,26|w|omega
cluyt|montano|montan root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
6,C,27,C,28|w|omega
melisso|meliss|myric root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
6,C,27,C,28,C,29,C,30|w|omega
laccero|laccer root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
6,C,27,C,28,C,29,C,30,C,31,C,32|w|omega
acroleine|acrolein root root C,1,(=,x,O,x,),x,C,2|a|alpha,=,x,C,3|b|beta|w|omega
methacrolein root root C,1,(=,x,O,x,),x,C,2|a|alpha,(C),x,=,x,C,3|b|beta|w|omega
acr root trivial C,1,(=,x,O,x,),x,C,2|a|alpha,=,x,C,3|b|beta|w|omega
hydracr root trivial C,1,(=,x,O,x,),x,C,2,C,3|w|omega,O,o

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methacr root trivial C,1,(=,x,O,x,),x,C,2,(,x,C,4,),x,=,x,C,3|w|omega
propiol root trivial C,1,(=,x,O,x,),x,C,2,#,x,C,3
glyoxal root trivial C,1,(=,x,O,x,),x,C,2,=,x,O,x
oxalo|oxal root diacid C,1,(=,x,O,x,),x,C,4@2,=,x,O,x
oxamid|oxam root trivial C,1,(=,x,O,x,),x,C,2,(,x,N,n,),x,=,x,O,x
oxanil root trivial
C,1,(=,x,O,x,),x,C,2,(,x,N,n,c,1',Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Ring1
,),x,=,x,O,x
mucochlor root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(Cl),x,=,x,C,3|b|beta|w|omega,(Cl),x,C=O,x
mucobrom root trivial
C,1,(=,x,O,x,),x,C,2|a|alpha,(Br),x,=,x,C,3|b|beta|w|omega,(Br),x,C=O,x
pyromuc root root C,x,c,x,Ring,Ring1,c,x,c,x,c,x,o,x,Ring,Ring1
malono|malon root diacid C,1,(=,x,O,x,),x,C,2|w|omega,C,4@3,=,x,O,x
tartrono|tartron root diacid C,1,(=,x,O,x,),x,C,2,(,x,O,x,),x,C,4@3,=,x,O,x
mesoxal root diacid C,1,(=,x,O,x,),x,C,2,(=,x,O,x,),x,C,4@3,=,x,O,x
mesoxalo root root C,4@1,(=,x,O,x,),x,C,2,(=,x,O,x,),x,C,3,(,x,O,x,),x,=,x,O,x
oxalacet root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3,(=,x,O,x,),x,C,4@4|w|omega,=,x,O,x
oxalaceto root diacid
C,4@1,(=,x,O,x,),x,C,2|a|alpha,C,3,(=,x,O,x,),x,C,4,(,x,O,x,),x,=,x,O,x
succino|succin root diacid C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4@4,=,x,O,x
isosuccino|isosuccin root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,(,x,C,3|b|beta,),x,C,4@4,=,x,O,x
caron root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,(C(C)(C),x,Ring,Ring1,),x,C,3|b|beta,Ring,Ring1,C,4
@4,=,x,O,x
male|malen|malein|toxil root diacid
C,1,(=,x,O,x,),x,/,x,C,2,=,x,C,3,\,x,C,4@4,=,x,O,x
fumar|bolet root diacid C,1,(=,x,O,x,),x,/,x,C,2,=,x,C,3,/,x,C,4@4,=,x,O,x
maleur root trivial C,1,(=,x,O,x,),x,/,x,C,2,=,x,C,3,\,x,C,4,N,x,C,x,(=O),x,N,x
citracon root diacid C,1,(=,x,O,x,),x,/,x,C,2,(C),x,=,x,C,3,\,x,C,4@4,=,x,O,x
mesacon root diacid C,1,(=,x,O,x,),x,/,x,C,2,(C),x,=,x,C,3,/,x,C,4@4,=,x,O,x
teracon root diacid C,1,(=,x,O,x,),x,C,2,(=C(C)C),x,C,3,C,4@4,=,x,O,x
mal root diacid C,1,(=,x,O,x,),x,C,2,(,x,O,x,),x,C,3,C,4@4,=,x,O,x
citramal root diacid C,1,(=,x,O,x,),x,C,2,(,x,O,x,)(,x,C,x,),x,C,3,C,4@4,=,x,O,x
pyrotartr|pyrotartar root diacid
C,1,(=,x,O,x,),x,C,2,(,x,C,x,),x,C,3,C,4@4,=,x,O,x
itacon root diacid C,1,(=,x,O,x,),x,C,2,(=,x,C,x,),x,C,3,C,4@4,=,x,O,x
tartar|tartr|dtartar|dtartr|uv|mesotartar|mesotartr pseudosugar unknown x,x
tartar|tartr|uv root diacid
C,1,(=O),x,Ring,Ring1,.,x,O,o,Ring,Ring2,.,x,O,o',Ring,Ring3,.,x,C,2,Ring,Ring1,
Ring,Ring2,C,3,Ring,Ring3,C,4@4,=,x,O,x
dtartar|dtartr root diacid
C,1,(=O),x,Ring,Ring1,.,x,O,o,Ring,Ring2,.,x,O,o',Ring,Ring3,.,x,[C@H],2,Ring,Ri
ng1,Ring,Ring2,[C@H],3,Ring,Ring3,C,4@4,=,x,O,x
ltartar|ltartr root diacid
C,1,(=O),x,Ring,Ring1,.,x,O,o,Ring,Ring2,.,x,O,o',Ring,Ring3,.,x,[C@@H],2,Ring,R
ing1,Ring,Ring2,[C@@H],3,Ring,Ring3,C,4@4,=,x,O,x
mesotartar|mesotartr root diacid
C,1,(=O),x,Ring,Ring1,.,x,O,o,Ring,Ring2,.,x,O,o',Ring,Ring3,.,x,[C@@H],2,Ring,R
ing1,Ring,Ring2,[C@H],3,Ring,Ring3,C,4@4,=,x,O,x
him root diacid
C,x,(=,x,O,x,),x,C,2,Ring,Ring1,C,3,(,x,C,4,Ring,Ring2,C,5,=,x,C,6,C,1,(,x,C,7,R
ing,Ring2,),x,Ring,Ring1,),x,C,4@x,=,x,O,x
glutaro|glutar root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,4@5,=,x,O,x

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adipo|adip root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,4@6,=,x,O,x
glutacon|glutacono root diacid C,1,(=,x,O,x,),x,C,2,=,x,C,3,C,4,C,4@5,=,x,O,x
mucon|mucono root diacid C,1,(=,x,O,x,),x,C,2,=,x,C,3,C,4,=,x,C,5,C,4@6,=,x,O,x
dihydromucon|dihydromucono root diacid
C,1,(=,x,O,x,),x,C,2,=,x,C,3,C,4,C,5,C,4@6,=,x,O,x
pimelo|pimel|piler root diacid
C,1,(=,x,O,x,),x,C,2,C,3,C,4,C,5,C,6,C,4@7,=,x,O,x
subero|suber root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,4@8,=,
x,O,x
azela|azele|azel|lepargyl root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,4@
9,=,x,O,x
sebaco|sebac root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,
C,4@10,=,x,O,x
traumat|traumato root diacid
C,1,(=,x,O,x,),x,C,2,=,x,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,4@12,=,x,O,x
brassylo|brassyl root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,
C,10,C,11,C,12,C,4@13,=,x,O,x
thapso|thaps root diacid
C,1,(=,x,O,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,
C,10,C,11,C,12,C,13,C,14,C,15,C,4@16,=,x,O,x
floion|phloion root diacid
C,1,(=,x,O,x,),x,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,(O),x,C,10,(O),x,C,11,C,12,C,13
,C,14,C,15,C,16,C,17,C,4@18,=,x,O,x
folin root diacid
C,x,(=,x,O,x,),x,(C(CC,x,C,4@x,=O)NC(C(C=C3)=CC=C3NCC(CN2)N(C=O)C1=C2N=C(N)NC1=O
)=O),x
spiculspor root diacid
C,x,(=,x,O,x,),x,Ring,Ring1,.,x,C,1,(,x,=,x,O,x,),x,(,x,O,x,Ring,Ring2,),x,C,2,C
,3,C,4,Ring,Ring2,Ring,Ring1,C,5,(,x,C,4@x,=,x,O,x,),x,C,6,C,7,C,8,C,9,C,10,C,11
,C,12,C,13,C,14,C,15
chaulmoogr root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,[C@@H],x,Ring,Ring1,c,x,c,x,C,x,C,x,Ring,Ring1
pyrocarbon root diacid C,x,(=,x,O,x,),x,O,x,C,4@x,=,x,O,x
imidodicarbon|iminodicarbon root diacid C,x,(=,x,O,x,),x,N,n,C,4@x,=,x,O,x
pyrocarbon root diacid C,x,(=,x,O,x,),x,O,x,C,4@x,=,x,O,x
thiodicarbon root diacid C,x,(=,x,O,x,),x,S,x,C,4@x,=,x,O,x
peroxydicarbon root diacid C,x,(=,x,O,x,),x,OO,x,C,4@x,=,x,O,x
thioperoxydicarbon root diacid C,x,(=,x,O,x,),x,SS,x,C,4@x,=,x,O,x
chelidon|chelid root diacid C,x,(=,x,O,x,),x,c1cc(=O)cc(o1),x,C,4@x,=,x,O,x
pamo|embon root diacid
C,x,(=,x,O,x,),x,C1=CC3=C(C=CC=C3)C(CC2=C(C=CC=C4)C4=CC(,x,C,4@x,=,x,O,x,)=C2O)=
C1O,x
citr root polyacid C,1,C,2,C,3,(,x,O,x,),x,(,x,C,x,),x,C,x,C,x
isocitr root polyacid C,x,C,x,(,x,O,x,),x,C,x,(,x,C,x,),x,C,x,C,x
tricarballyl root polyacid C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x
aconit root polyacid C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x
trimellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,c,5,(,x,C,x,),x,c,6,Ring,Ring1
hemimellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,(,x,C,x,),x,c,4,c,5,c,6,Ring,Ring1

hemimellitene root root
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,(,x,C,x,),x,c,4,c,5,c,6,Ring,Ring1
pyromellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,(,x,C,x,),x,c,5,(,x,C,x,),x,c,6,Ring,
Ring1
pyromellitene root root
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,(,x,C,x,),x,c,5,(,x,C,x,),x,c,6,Ring,
Ring1
mellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(C),x,c,3,(C),x,c,4,(C),x,c,5,(C),x,c,6,(C),x,Ring,Ring1
trimes root polyacid
C,x,c,1,Ring,Ring1,c,2,c,3,(,x,C,x,),x,c,4,c,5,(,x,C,x,),x,c,6,Ring,Ring1
mellophan root polyacid
C,x,c,1,Ring,Ring1,c,2,(C),x,c,3,(C),x,c,4,(C),x,c,5,c,6,Ring,Ring1
prehnit root polyacid
C,x,c,1,Ring,Ring1,c,2,(C),x,c,3,(C),x,c,4,c,5,(C),x,c,6,Ring,Ring1
berberon|beron root polyacid
C,x,c,2,Ring,Ring1,c,3,(,x,C,x,),x,c,4,c,5,(,x,C,x,),x,c,6,n,1,Ring,Ring1
phthalide root root
O,x,=,x,C,1,Ring,Ring1,O,2,C,3|a|alpha,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring
,Ring1,Ring,Ring2
phthalane|phthalan root root
C,1,Ring,Ring1,O,2,C,3,C,3a,Ring,Ring2,=,x,C,4,C,5,=,x,C,6,C,7,=,x,C,7a,Ring,Rin
g1,Ring,Ring2
phthalo|phthal|orthophthal root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,(,x,C,4@x,=,x,O,x,),x,c,3,c,4,c,5,c,6,Ring,R
ing1
homophthalo|homophthal root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,(,x,C,x,C,4@x,=,x,O,x,),x,c,3,c,4,c,5,c,6,Ri
ng,Ring1
isophthalo|mphthalo|isophthal|mphthal root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,c,3,(,x,C,4@x,=,x,O,x,),x,c,4,c,5,c,6,Ring,R
ing1
terephthalo|pphthalo|terephthal|pphthal root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,C,4@x,=,x,O,x,),x,c,5,c,6,Ring,R
ing1
uvit root diacid
C,x,(=,x,O,x,),x,c,1,Ring,Ring1,c,2,c,3,(,x,C,4@x,=,x,O,x,),x,c,4,c,5,(C),x,c,6,
Ring,Ring1
leucate|leucicacid root root
C,1,(=,x,O,x,),x,(,x,O,1@x,),x,C,2,(,x,O,x,),x,C,3,C,4,(,x,C,5,),x,C,x
phenylephrine|phenylephrin root root Oc1cccc(C(O)CNC)c1,x
norepinephrine|norepinephrin|noradrenaline|noradrenalin|arterenol root root
Oc1cc(C(O)CN)ccc1O,x
epinephrine|epinephrin|adrenaline|adrenalin root root Oc1cc(C(O)CNC)ccc1O,x
adrenalone root root O=C(CNC)c1ccc(O)c(O)c1,x
norephedrine|norephedrin root root
OC(C(,x,N,n,)C),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
ephedrine|ephedrin|pseudoephedrine|pseudoephedrin root root
OC(C(,x,N,n,C)C),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
taurine|taurin root root O,1@x,S,x,(=O)(=O),x,C,1,C,2,N,n
hypotaurine|hypotaurin root root O,1@x,S,x,(=O),x,C,1,C,2,N,n
cadaverine|cadaverin root root N,n,C,1,C,2,C,3,C,4,C,5,N,n'
putrescine|putrescin root root N,n,C,1,C,2,C,3,C,4,N,n'

albizzi aminoacid ine
C,1,Ring,Ring1,.,,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,NC(=O)N,x

alan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta
homoalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|d|delta|w
|omega
alanos aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,N,x,(,x,O,x,)
,x,N,x,=,x,O,x
alloisoleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@@H],3|b|beta,(,x,
C,4|g|gamma,C,5|d|delta,),x,C,3',
allothreono|allothreon aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@H],3|b|beta,(,x,C
,4|g|gamma,),x,O,x
allys aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,=O,x
argin aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,N,nd|ndelta,C,x,(=,x,N,nw'|nomega',),x,N,nw|nomega|ngamma
asparag aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,(
=,x,O,x,),x,N,ngamma
aspart aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3,C,4|g|gamma|b|beta,(
=,x,O,x,),x,O,x
azaser aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,O,x,C(=O)C=[N
+]=[N-],x
betaalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nbeta|n3,C,2|a|alpha,C,3|b|beta,Ring,Ring1
buthion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,x,CCCC,x
canavan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,O
NC(=N)N,x
carbocyste aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s,CC(=O),x,
O,1@x
citrull aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,N,x,C,x,(=,x,O,x,),x,N,x
cycloleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,Ring,Ring2,C,3|b|beta,C,
4|g|gamma,C,5|d|delta,C,6,Ring,Ring2
cyste reqineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s
cyste aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s,(=O)(=O),
x,O,1@x,
ethion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,x,C,x,C,x
isoglutam reqineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,Ring,Ring2,.,x,C,2|a|alpha,Ring,Ring1,C,3|b|bet
a,C,4|g|gamma,Ring,Ring2,C,5|d|delta,(=,x,O,x,),x,N,x

glutam reqineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,(=,x,O,x,),x,N,nd|ndelta|n5
glutam aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,(=,x,O,x,),x,O,1@x
glyc aminoacid ine C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1
histid aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,c,4,Ring,Ring2,c,
5,n,1|nt|ntau|im|nim|n'|tau|prefhydro,c,2,n,3|np|npi,Ring,Ring2
homoargin aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,N,nd|ndelta,C,x,(=,x,N,nw'|nomega',),x,N,nw|nomega
homocitrull aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,N,x,C,x,(=,x,O,x,),x,N,x
homocyste reqineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,s
homocyste aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,s,(=O)(=O),x,O,1@x
homoglutam reqineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,(=,x,O,x,),x,N,ne|nepsilon|n6
homophenylalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Rin
g,Ring2,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring2
homoprol aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,C,5,C,6,Rin
g,Ring2
homoser aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,O
,x
homotryptoph aminoacid ane
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,g|gamma,C,3,Rin
g,Ring2,=,x,C,2,N,1,C,7a,Ring,Ring3,=,x,C,7,C,6,=,x,C,5,C,4,=,x,C,3a,Ring,Ring2,
Ring,Ring3
iboten aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C2=CC(=O)NO2,x
isoleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@H],3|b|beta,(,x,C
,4|g|gamma,C,5|d|delta,),x,C,3',
isoser aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,Ring,Ring2,.,x,C,2|a|alpha,Ring,Ring1,(O),x,C,3
|b|beta,Ring,Ring2
isoval aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,(,x,C,2',),x,Ring,Ring1,C,3|b|beta,
C,4|g|gamma
kynuren aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C(=O),x,c,1,Ring,
Ring2,c,2,(N),x,c,3,c,4,c,5,c,6,Ring,Ring2
leuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,(
,x,C,5|d|delta,),x,C,5'

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lys aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,N,n6|nw|nomega|nepsilon|ne|nz|n'
methion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,x,C,x
mimos aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,N2C=C(O)C(=O)
C=C2,x
norleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon
norval aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta
ornith aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,N,n5|ndelta|nd
penicillam aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,(C)(C)S,x
phenylalan|3phenylalan|betaphenylalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,c,x,Ring,Ring2,c,
2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring2
prol aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,C,5,Ring,Ri
ng2
3hydroxyprol|hydroxyprol aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,(O),x,C,4,C,5,R
ing,Ring2
4hydroxyprol aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,(O),x,C,5,R
ing,Ring2
5hydroxyprol aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,C,5,(O),x,R
ing,Ring2
pyroglutam aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,C,5,(=O),x,
Ring,Ring2
sarcos aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,(,x,C,2|a|alpha,Ring,Ring1,),x,C,x
selenocyste reqineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,[Se],se
selenomethion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,[
Se],x,C,x
ser aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,O,x
tleuc|tertleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,(,x,C,3',)(,x
,C,3'',),x,C,3'''
theano|thean aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,x,(=O),x,N,x,C,x,C,x
thiocitrull aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,N,x,C,x,(=,x,S,x,),x,N,x

threono|threon aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@@H],3|b|beta,(,x,
C,4|g|gamma,),x,O,x
tryptoph aminoacid ane
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,3,Ring,Ring2,=,
x,C,2,N,1,C,7a,Ring,Ring3,=,x,C,7,C,6,=,x,C,5,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
thyron aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2|ortho,C,3|m|meta,=,x,C,4,(,x,O,x,C,1',Ring,Ring3,=,x,C,2',C,3',=,x,C,4',(,
x,O,x,),x,C,5',=,x,C,6',Ring,Ring3,),x,C,5,=,x,C,6,Ring,Ring2
thyrox aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2|ortho,C,3|m|meta,(I),x,=,x,C,4,(,x,O,x,C,1',Ring,Ring3,=,x,C,2',C,3',(I),x
,=,x,C,4',(,x,O,x,),x,C,5',(I),x,=,x,C,6',Ring,Ring3,),x,C,5,(I),x,=,x,C,6,Ring,
Ring2
tyros|ptyros|paratyros aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2|ortho,C,3|m|meta,=,x,C,4,(,x,O,x,),x,C,5,=,x,C,6,Ring,Ring2
mtyros|metatyros aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2|ortho,C,3|m|meta,(,x,O,x,),x,=,x,C,4,C,5,=,x,C,6,Ring,Ring2
orthotyros aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2|ortho,(,x,O,x,),x,C,3|m|meta,=,x,C,4,C,5,=,x,C,6,Ring,Ring2
val aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,(,x,C,4|g|gam
ma,),x,C,4'|5
willardi aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,n2ccc(=O)nc(=
O)2,x
djenkol aminodiacid ine
C,1,(=,x,O,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
S,x,C,x,S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=,x,O,x
cyst aminodiacid ine
C,1,(=,x,O,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
S,x,S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=,x,O,x
cystathion aminodiacid ine
C,1,(=,x,O,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
C,4|g|gamma,S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=,x,
O,x
homocyst aminodiacid ine
C,1,(=,x,O,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
C,4|g|gamma,S,x,S,x,C,4'|g'|gamma',C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nal
pha',),x,C,4@x,=,x,O,x
lanthion aminodiacid ine
C,1,(=,x,O,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=,x,O,x
selenocyst aminodiacid ine
C,1,(=,x,O,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
[Se],x,[Se],x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=,x,O,
x
selenocystathion aminodiacid ine
C,1,(=,x,O,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
C,4|g|gamma,[Se],x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=
,x,O,x
in|ine enderaminoacid ine O,8@x,.,x,O,5@x
an|ane enderaminoacid ane O,8@x,.,x,O,5@x

yl enderaminoacid yl O,8@x
ol enderaminoacid suffix O,8@x
aceglutamide|aceglutamid root root O=C(,x,O,1@x,)C(NC(C)=O)CCC(N)=O,x
methionol root root CSCCCO,x
tryptophol root root
OCC,x,c,3,Ring,Ring1,c,2,n,1,c,7a,Ring,Ring2,c,7,Ring,Ring1,c,6,c,5,c,4,c,3a,Rin
g,Ring2

cysteamine|cysteamin root root N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,s
histamine|histamin root root
N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,4,Ring,Ring2,=,x,C,5,N,1|nt|ntau,C,2,=
,x,N,3|np|npi,Ring,Ring2
methioninamine|methioninamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,C,x
tryptamine|tryptamin root root
N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,7a,Ring,Rin
g3,=,x,C,7,C,6,=,x,C,5,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
melatonin root root
N,n|nalpha|n2|nomega,(C(=O)C),x,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,
7a,Ring,Ring3,=,x,C,7,C,6,=,x,C,5,(OC),x,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
serotonin root root
N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,7a,Ring,Rin
g3,=,x,C,7,C,6,=,x,C,5,(O),x,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
tyramine|tyramin|tyrosamine|tyrosamin root root
N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,1,Ring,Ring2,=,x,C,2|ortho,C,3|m|meta,
=,x,C,4,(,x,O,x,),x,C,5,=,x,C,6,Ring,Ring2
cystamine|cystamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,S,x,C,3'|b'|beta',C,2'|a'|alpha'
,N,n'|na'|nalpha'
selenocystamine|selenocystamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,[Se],x,[Se],x,C,3'|b'|beta',C,2'|a'|
alpha',N,n'|na'|nalpha'
cystathionamine|cystathionamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,C,3'|b'|beta',C,2'|a
'|alpha',N,n'|na'|nalpha'
homocystamine|homocystamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,S,x,C,4'|g'|gamma',C
,3'|b'|beta',C,2'|a'|alpha',N,n'|na'|nalpha'
lanthionamine|lanthionamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,C,3'|b'|beta',C,2'|a'|alpha',N,n
'|na'|nalpha'
methional root root O,x,=,x,C,1,C,2,C,3,S,x,C,x

glycero sugar hexose O,x,=,x,C,1,[C@H](,2,O,x,),x,C,3,O,x
erythro|erythr sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,C,4,O,x
threo|thre sugar hexose O,x,=,x,C,1,[C@@H](,2,O,x,),x,[C@H](,3,O,x,),x,C,4,O,x
ribo|rib sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x
arabino|arabin|arab sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x
xylo|xyl sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x
lyxo|lyx sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x

allo sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6
,O,x
altro|altr sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,
6,O,x
gluco|gluc sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,
6,O,x
manno|mann sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6,O,x
gulo|gul sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C,
6,O,x
ido sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6,O,x
galacto|galact|dulc sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6,O,x
talo|tal sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,
C,6,O,x
boivin sugar hexose
O,x,=,x,C,1,[C@H],2,[C@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C,6
digitox sugar hexose
O,x,=,x,C,1,C,2,[C@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6
oli sugar hexose
O,x,=,x,C,1,[C@H],2,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C,6
oliv sugar hexose
O,x,=,x,C,1,[C@H],2,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6
glucohept sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@H](,3,O,x,),x,[C@H](,4,O,x,),x,[C@@H](,5,O,x,)[C
@H](,6,O,x,),x,C,7,O,x

fuco|fuc sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
quinovo|quinov sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,
6
rhamno|rhamn sugar hexose
O,x,=,x,C,1,[C@@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
rhodeo|rhode sugar hexose
O,x,=,x,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
thymino|thymin sugar hexose
O,x,=,x,C,1,[C@H],2,[C@H](,3,O,x,),x,[C@H](,4,O,x,),x,C,5,O,x
galactosamine|galactosamin|chondrosamine|chondrosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6,O,x
glucosamine|glucosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,
6,O,x

mannosamine|mannosamin sugar trivial
O,x,=,x,C,1,[C@@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6,O,x
fucosamine|fucosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
quinovosamine|quinovosamin sugar trivial
O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,
6
rhamnosamine|rhamnosamin sugar trivial
O,x,=,x,C,1,[C@@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C
,6
glucal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x
rhamnal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6
galactal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x
glucamine sugar trivial
N,n,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6,O,
x

sucr sugar disugar
OC[C@@]1([C@@H](O)[C@H](O)[C@H](O1)CO)O[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO
)O2,x
trehal sugar disugar
O[C@H]1[C@H](O)[C@@H](CO)O[C@H](O[C@H]2[C@@H](O)[C@H](O)[C@@H](O)[C@H](CO)O2)[C@
@H]1O,x
melezit sugar disugar
OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O[C@@]2(CO)[C@@H](O[C@H]3O[C@H](CO)[C@
@H](O)[C@H](O)[C@H]3O)[C@H](O)[C@@H](CO)O2)O1,x
stachy|lupe sugar disugar
O[C@H]1[C@@H](CO)O[C@H](OC[C@H]2O[C@H](O[C@H]3[C@@H](O[C@]4(CO)O[C@H](CO)[C@@H](
O)[C@@H]4O)O[C@H](CO)[C@@H](O)[C@@H]3O)[C@H](O)[C@@H](O)[C@H]2O)[C@H](O)[C@H]1O,
x
lact sugar disugar
OC[C@H]1O[C@@H](O[C@@H]([C@H](O)[C@@H](O)[C@@H](O)O2)[C@H]2CO)[C@H](O)[C@@H](O)[
C@H]1O,x
malt|maltobi sugar disugar
O[C@@H]1[C@@H](O)[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](O)O[C@@H]2CO)O[C@H](CO)[C
@H]1O,x
maltotri sugar disugar
O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@@H]1O[C@@H]2[C@@H](CO)O[C@H](O[C@@H]3[C@@
H](CO)OC(O)[C@H](O)[C@H]3O)[C@H](O)[C@H]2O,x
maltotetra sugar disugar
O[C@@H]([C@@H](O[C@H]4[C@H](O)[C@H]([C@@H](O)O[C@@H]4CO)O)O[C@@H]1CO)[C@@H](O)[C
@@H]1O[C@@H]2[C@H](O)[C@H]([C@H](O[C@@H](O[C@H](CO)[C@H]3O)[C@H](O)[C@H]3O)[C@@H
](CO)O2)O,x
maltopenta sugar disugar
O[C@H]([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@@H]1[C@@H](CO)O[C@H](O[C@H]3[C@H](O)[
C@H]([C@@H](O[C@H]4[C@H](O)[C@H]([C@@H](O[C@H]5[C@H](O)[C@H]([C@@H](O)O[C@@H]5CO
)O)O[C@@H]4CO)O)O[C@@H]3CO)O)[C@H](O)[C@H]1O,x
maltohexa sugar disugar
O[C@@H]([C@@H](O[C@H]3[C@H](O)[C@H]([C@@H](O[C@H]6[C@H](O)[C@H]([C@@H](O)O[C@@H]
6CO)O)O[C@@H]3CO)O)O[C@@H]1CO)[C@@H](O)[C@@H]1O[C@@H]2[C@H](O)[C@H]([C@H](O[C@@H
]4[C@H](O)[C@H]([C@H](O[C@@H](O[C@H](CO)[C@H]5O)[C@H](O)[C@H]5O)[C@@H](CO)O4)O)[
C@@H](CO)O2)O,x

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melibi sugar disugar
O[C@H]1[C@@H](OC[C@H](([C@@H](O)[C@H](O)[C@H]2O)O[C@H]2O)O[C@H](CO)[C@H](O)[C@@H]1O,x
cellobi sugar disugar
OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@H](O[C@@H]2[C@@H](CO)O[C@@H](O)[C@H](O)[C@H]2O)O1,x
cellotri sugar disugar
O[C@H]([C@H]1O)[C@H](O[C@H]2[C@H](O)[C@H]([C@H](O[C@H]3[C@H](O)[C@H](C(O)O[C@@H]3CO)O)O[C@@H]2CO)O)O[C@H](CO)[C@H]1O,x
cellotetra sugar disugar
OC(O[C@@H](CO)[C@@H]1O[C@H]2[C@@H](O)[C@H](O)[C@@H](O[C@@H]3[C@@H](O)[C@H](O)[C@H](O[C@@H]4[C@H](O)[C@H](O)[C@@H](O)[C@H](CO)O4)[C@H](CO)O3)[C@H](CO)O2)[C@@H](O)[C@@H]1O,x
cellopenta sugar disugar
OC(O[C@H]1CO)[C@@H](O)[C@@H](([C@H]1O[C@H]2[C@@H](O)[C@H](O)[C@@H](O[C@H](O[C@@H](CO)[C@@H]3O[C@@H]4[C@@H](O)[C@H](O)[C@@H](O[C@@H]5[C@@H](O)[C@H](O)[C@@H](O)[C@H](CO)O5)[C@H](CO)O4)[C@@H](O)[C@@H]3O)[C@H](CO)O2)O,x
chitobi sugar disugar
N,n,[C@@H](([C@H](O)O[C@@H]2CO)[C@@H](O)[C@@H]2O[C@H](O1)[C@H](,x,N,n',)[C@@H](O)[C@H](O)[C@H]1CO,x
chitotri sugar disugar
N,n,[C@@H](C(O)O[C@@H]3CO)[C@@H](O)[C@@H]3O[C@H](O[C@@H]1CO)[C@H](,x,N,n',)[C@@H](O)[C@@H]1O[C@H](O[C@H](CO)[C@H]2O)[C@H](,x,N,n'',)[C@H]2O,x
raffin|melit|melitri sugar disugar
OC[C@H]1OC(OC[C@H]2OC(O[C@@]3(CO)[C@@H](O)[C@H](O)[C@@H](CO)O3)[C@H](O)[C@@H](O)[C@@H]2O)[C@H](O)[C@@H](O)[C@H]1O,x
gentiobi sugar disugar
O[C@H]1[C@H](OC[C@H](([C@@H](O)[C@H](O)[C@H]2O)O[C@H]2O)O[C@H](CO)[C@@H](O)[C@@H]1O,x
palatin sugar disugar
OC[C@@]1(O)O[C@H](CO[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)[C@@H](O)[C@@H]1O,x
turan sugar disugar
O[C@H](([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@@H]1C(O)(CO)OC[C@@H](O)[C@H]1O,x
ose endersugar ose x,x
itol endersugar itol x,x
ityl endersugar makefree x,x
ide|id|oside|osid endersugar oside x,x
on|ono endersugar on x,x
uron|urono endersugar uron x,x
ar|aro endersugar ar x,x
odialdo|odiald endersugar dialdo x,x
oxirose|oxiros pyranose unknown 2,x
oxetose|oxetos pyranose unknown 3,x
furanose|furanos|ofuranose|ofuranos pyranose unknown 4,x
pyranose|pyranos|opyranose|opyranos pyranose unknown 5,x
septanose|septanos|oseptanose|oseptanos pyranose unknown 6,x
tetro multsugar unknown 4,x
pento multsugar unknown 5,x
hexo multsugar unknown 6,x
hepto multsugar unknown 7,x
octo multsugar unknown 8,x
nono multsugar unknown 9,x
deco multsugar unknown 10,x
ulo|ul structsugarender ulose C=O,x
osamine structsugarender osamine N,x
deoxy|desoxy deoxy unknown C,x

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inositol pseudosugar unknown x,x
inositol root root OC1C(O)C(O)C(O)C(O)C1O,x
mesoinositol|myoinositol root root
O,x,[C@H],1,Ring,Ring1,[C@@H],2,(O),x,[C@@H],3,(O),x,[C@H],4,(O),x,[C@@H],5,(O),
x,[C@@H],6,Ring,Ring1,O,x
scylloinositol root root
O,x,[C@H],1,Ring,Ring1,[C@H],2,(O),x,[C@@H],3,(O),x,[C@H],4,(O),x,[C@@H],5,(O),x
,[C@@H],6,Ring,Ring1,O,x
epiinositol root root
O,x,[C@H],1,Ring,Ring1,[C@@H],2,(O),x,[C@@H],3,(O),x,[C@@H],4,(O),x,[C@@H],5,(O)
,x,[C@@H],6,Ring,Ring1,O,x
dinositol root root O[C@H]1[C@@H](O)[C@H](O)[C@H](O)[C@@H](O)[C@@H]1O,x
linositol root root O[C@@H]1[C@H](O)[C@@H](O)[C@@H](O)[C@H](O)[C@H]1O,x
quebrachitol root root O[C@@H]1[C@H](O)[C@@H](O)[C@@H](OC)[C@H](O)[C@H]1O,x
muram pseudosugar unknown x,x
muram root root
CC(C)O,x,[C@H],3,Ring,Ring1,[C@H],4,(O),x,[C@@H],5,(,x,C,6,O,x,),x,O,x,[C@H],1,(
O),x,[C@H],2,(,x,N,n,),x,Ring,Ring1
neuramin pseudosugar unknown x,x
neuramin root root
C,x,[C@@],2,Ring,Ring1,(O),x,O,x,[C@@H],6,(,x,[C@H],7,(O),x,[C@H],8,(O),x,C,9,O,
x,),x,[C@H],5,(,x,N,n,),x,[C@@H],4,(O),x,C,3,Ring,Ring1
sial pseudosugar unknown x,x
sial root root
C,x,[C@@],2,Ring,Ring1,(O),x,O,x,[C@@H],6,(,x,[C@H],7,(O),x,[C@H],8,(O),x,C,9,O,
x,),x,[C@H],5,(,x,NC(=O)C,x,),x,[C@@H],4,(O),x,C,3,Ring,Ring1

adenos|adenyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(,x,N,n|n6,),x,n,1,c,2,n,3
,c,4,Ring,Ring3,Ring,Ring2
cytid|cytidyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3,c,4,(,x,N,n|n4,),x,c,5,c,6,Ring,Ring2
guanos|guanyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(=O),x,N,1,c,2,(,x,N,n|n2,
),x,n,3,c,4,Ring,Ring3,Ring,Ring2
inos nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(O),x,n,1,c,2,n,3,c,4,Ring
,Ring3,Ring,Ring2
thymid|thymidyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,C,2',[C@@H],1',(O,x,Ring,Ring1,),x
,n,1,Ring,Ring2,c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,(C),x,c,6,Ring,Ring2
urid|uridyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,c,6,Ring,Ring2
xanthos|xanthoyl|xanthonyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(O),x,n,1,c,2,(O),x,n,3,c,
4,Ring,Ring3,Ring,Ring2
orotid|orotidyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3,c,4,(=O),x,c,5,c,6,(C(=O)O),x,Ring,Rin
g2

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cordycep nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring
1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(,x,N,n|n6,),x,n,1,c,2,n,3,c,4,R
ing,Ring3,Ring,Ring2

adenyl loveracid root
P,x,(=O),x,(,x,O,1@o',),x,(,x,O,1@o,),x,O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,R
ing,Ring3,c,6,(,x,N,n|n6,),x,n,1,c,2,n,3,c,4,Ring,Ring3,Ring,Ring2
cytidyl loveracid root
P,x,(=O),x,(,x,O,1@o',),x,(,x,O,1@o,),x,O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,
3,c,4,(,x,N,n,),x,c,5,c,6,Ring,Ring2
guanyl loveracid root
P,x,(=O),x,(,x,O,1@o',),x,(,x,O,1@o,),x,O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,R
ing,Ring3,c,6,(=O),x,n,1,c,2,(,x,N,n|n2,)n,3,c,4,Ring,Ring3,Ring,Ring2
inos loveracid root
P,x,(=O),x,(,x,O,1@o',),x,(,x,O,1@o,),x,O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,R
ing,Ring3,c,6,(O),x,n,1,c,2,n,3,c,4,Ring,Ring3,Ring,Ring2
thymidyl loveracid root
P,x,(=O),x,(,x,O,1@o',),x,(,x,O,1@o,),x,O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,C,2',[C@@H],1',(O,x,Ring,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,3|n,c,4,(=O
),x,c,5,(C),x,c,6,Ring,Ring2
uridyl loveracid root
P,x,(=O),x,(,x,O,1@o',),x,(,x,O,1@o,),x,O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,
3|n,c,4,(=O),x,c,5,c,6,Ring,Ring2
xanthoyl|xanthonyl loveracid root
P,x,(=O),x,(,x,O,1@o',),x,(,x,O,1@o,),x,O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,R
ing,Ring3,c,6,(O),x,n,1,c,2,(O),x,n,3,c,4,Ring,Ring3,Ring,Ring2

purineriboside root root
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,n,1,c,2,n,3,c,4,Ring,Ring3
,Ring,Ring2
thuj root root
C,3,Ring,Ring1,C,2,C,1,Ring,Ring2,(,x,C,7,(,x,C,8,),x,C,9,),x,C,6,C,5,Ring,Ring2
,C,4,Ring,Ring1,(,x,C,10,),x
car root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,(,x,C,4,C,5,C,6,Ring,Ring1,(,x,C,7,Ring,Ring2,
(,x,C,8,),x,C,9,),x,),x,C,10
norcar root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,C,5,C,6,Ring,Ring1,(,x,C,7,Ring,Ring2,),x
pin root root
C,2,Ring,Ring1,(,x,C,10,),x,C,3,C,4,C,5,(,x,C,7,Ring,Ring2,),x,C,6,(,x,C,8,)(,x,
C,9,),x,C,1,Ring,Ring2,Ring,Ring1
norpin root root
C,2,Ring,Ring1,C,3,C,4,C,5,(,x,C,7,Ring,Ring2,),x,C,6,C,1,Ring,Ring2,Ring,Ring1
camphor loveracid root
C,10,C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,(,x,C,
8,),x,(,x,C,9,),x,Ring,Ring2
camphor root root
C,10,C,1,Ring,Ring1,Ring,Ring2,C,2,(=O),x,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7
,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2

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norcamphor root root

C,1,Ring,Ring1,Ring,Ring2,C,2,(=O),x,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,Ring
,Ring2

camphorquinone|camphoroquinone root root

C,10,C,1,Ring,Ring1,Ring,Ring2,C,2,(=O),x,C,3,(=O),x,C,4,(,x,C,5,C,6,Ring,Ring1,
),x,C,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2

borne|born|camphane|camphan|bornylane|bornylan|isoborne|isoborn root root

C,2,Ring,Ring1,C,3,C,4,Ring,Ring2,C,5,C,6,C,1,Ring,Ring1,(,x,C,7,Ring,Ring2,(,x,
C,8,),x,C,9,),x,C,10

camphan loveracid root

C,1,Ring,Ring1,Ring,Ring2,O,2,C,3,(=O),x,C,4,(,x,C,5,C,6,Ring,Ring1,),x,(,x,C,7,
(,x,C,x,)(,x,C,x,),x,Ring,Ring2,),x,C,x

norborne|norborn|norborna root root

C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,Ring,Ring2

norbornadien|norbornadiene|25norbornadien|25norbornadiene root root

C,1,Ring,Ring1,Ring,Ring2,C,2,=,x,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,C,7,Rin
g,Ring2

norbornen|norbornene|2norbornen|2norbornene root root

C,1,Ring,Ring1,Ring,Ring2,C,2,=,x,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,Ring,Ri
ng2

5norbornen|5norbornene root root

C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,C,7,Ring,Ri
ng2

camphene|camphen root root

C,1,Ring,Ring1,Ring,Ring2,C,2,(,x,C,x,),x,(,x,C,x,),x,C,3,(,x,=,x,C,x,),x,C,4,(,
x,C,5,C,6,Ring,Ring1,),x,C,7,Ring,Ring2

phosgene|phosgen root root ClC(=O)Cl,x

triphosgene|triphosgen root root C(Cl)(Cl)(Cl)OC(=O)OC(Cl)(Cl)(Cl),x

glyoxyl root root C,1,C,2|w|omega,=,x,O,x

pyruv root root C,1,C,2,(=,x,O,x,),x,C,3|w|omega

glycerol|snglycerol|racglycerol pseudosugar unknown x,x

glycerol|snglycerol|snglycero|racglycerol|racglycero|glycero|glycerine root root

O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma

glycerin root root O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma

glycerone|glyceron root root O,1@1|a|alpha,C,x,C,x,(=O),x,C,x,O,1@3|g|gamma

in|anoin glycerin root

O,1@1|a|alpha,C,x,C,x,(,x,O,1@2|b|beta,),x,C,x,O,1@3|g|gamma|a'|alpha'

gerani|geran root root

C,1,/,x,C,2,=,x,C,3,(,x,C,x,),x,/,x,C,4,C,5,C,6,=,x,C,7,(,x,C,x,),x,C,8

tetrahydrogerani|geran root root

C,1,C,2,C,3,(,x,C,x,),x,C,4,C,5,C,6,C,7,(,x,C,x,),x,C,8

ner root root

C,1,/,x,C,2,=,x,C,3,(,x,C,x,),x,\,x,C,4,C,5,C,6,=,x,C,7,(,x,C,x,),x,C,8

phyt root root

C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,C,x,(,x,C,x,),x,
C,x,C,x,C,x,C,x,(,x,C,x,),x,C,x

citral root root

O,x,=,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x

ethylcitral root root

O,x,=,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,=,x,C,x,(,x,C,x,),x,C,x,C,x

citronell|betacitronell|baran root root CCC(C)CCC=C(C)C,x

linalo root root C(CCC=C(C)C)(C=C)C,x

dihydrolinalo root root C(CCC=C(C)C)(CC)C,x

tetrahydrolinalo root root C(CCCC(C)C)(CC)C,x

lavandul root root CC(C(=C)C)CC=C(C)C,x

tetrahydrolavandul root root CC(C(C)C)CCC(C)C,x

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farnes root root
C,1,C,2,=,x,C,3,(C),x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8,C,9,C,10,=,x,C,11,(C)C,x
ocimene root root C,1,=,x,C,2,C,3,(C)=,x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8
alloocimene|allocimen root root
C,1,C,2,(C)=,x,C,3,C,4,=,x,C,5,(C),x,C,6,=,x,C,7,C,8
nerolid root root C(C)(C=C)CCC=C(C)CCC=C(C)C,x
all root root C,1|a|alpha,C,2|b|beta,=,x,C,3|g|gamma
isoall root root C,1|a|alpha,=,x,C,2|b|beta,C,3|g|gamma
homoall root root C,1|a|alpha,C,2|b|beta,C,3|g|gamma,=,x,C,4|d|delta
methall root root C,1,C,2,(,x,C,x,),x,=,x,C,3
triazeno root root N,4@1,=,x,N,2,N,3
vin root root C,1|a|alpha,=,x,C,2|b|beta
hydrazine|hydrazin root root N,1|n,N,2|n'
dithioiminocarbonate root root S,1@s,C,x,(=,x,N,n,),x,S,1@s'
urea|carbamide|carbamid root root N,1|n,C,2,(,x,=,x,O,o,),x,N,3|n'
sulfocarbamide|sulfocarbamid|sulfourea root root
N,1|n,C,2,(,x,=,x,S,s,),x,N,3|n'
biurea root root N,1,C,2,(=O),x,N,3,N,4,C,5,(=O),x,N,6
guanyl root root C,4@x,(=N),x,N,x
uronium root root N,1|n,C,2,(,x,N,3|n',),x,=,x,[O+],o
ureido root root N,4@1|n,C,2,(,x,=,x,O,o,),x,N,3|n'
ureylene|ureylen root bridge N,4@1|n,C,2,(,x,=,x,O,o,),x,N,4@3|n'
carbanilide|carbanilid root root
c,6,Ring,Ring1,c,5,c,4,c,3,c,2,c,1,Ring,Ring1,N,n,C,x,(,x,=,x,O,o,),x,N,n',c,1',
Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
tms root root [Si],4@x,(C)(C)(C),x
tbdms root root [Si],4@x,(C(C)(C)C)(C)(C),x
plumb root root [Pb],1
sil root root [Si],x
stann root root [Sn],x
bor root root [B],x
germ root root [Ge],x
amine|amin|ammonia root root N,n
phosphine|phosphin root root P,x
arsine|arsin root root [As],x
hydrogen root root [H],4@x
deuterium root root [2H],4@x
tritium root root [3H],4@x
hydrido root root [H-],4@x
deuterido root root [2H-],4@x
lithio root root [Li],4@x
sodio root root [Na],4@x
potassio|kalio root root [K],4@x
fluoro|fluor root root F,4@x
chloro|chlor root root Cl,4@x
chlorosyl root root Cl,4@x,=O,x
chloryl root root Cl,4@x,(=O)=O,x
perchloryl root root Cl,4@x,(=O)(=O)=O,x
borono root root [B],4@x,(O)O,x
lithium root metal [Li],x
sodium|natrium root metal [Na],x
potassium|kalium root metal [K],x
rubidium root metal [Rb],x
cesium root metal [Cs],x
francium root metal [Fr],x
beryllium|glucinium root metal [Be],x
magnesium root metal [Mg],x
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calcium root metal [Ca],x
strontium root metal [Sr],x
barium root metal [Ba],x
radium root metal [Ra],x
scandium root metal [Sc],x
yttrium root metal [Y],x
lanthanum root metal [La],x
cerium root metal [Ce],x
praesodymium|praseodymium root metal [Pr],x
neodymium root metal [Nd],x
promethium root metal [Pm],x
samarium root metal [Sm],x
europium root metal [Eu],x
gadolinium root metal [Gd],x
terbium root metal [Tb],x
dysprosium root metal [Dy],x
holmium root metal [Ho],x
erbium root metal [Er],x
thulium root metal [Tm],x
ytterbium root metal [Yb],x
lutetium|cassiopeium root metal [Lu],x
actinium root metal [Ac],x
thorium root metal [Th],x
protactinium root metal [Pa],x
uranium root metal [U],x
neptunium root metal [Np],x
plutonium root metal [Pu],x
americium root metal [Am],x
curium root metal [Cm],x
berkelium root metal [Bk],x
californium root metal [Cf],x
einsteinium root metal [Es],x
fermium root metal [Fm],x
mendelevium root metal [Md],x
nobelium root metal [No],x
lawrencium root metal [Lr],x
titanium root metal [Ti],x
zirconium root metal [Zr],x
hafnium root metal [Hf],x
vanadium root metal [V],x
niobium root metal [Nb],x
tantalum root metal [Ta],x
chromium root metal [Cr],x
molybdenum root metal [Mo],x
tungsten root metal [W],x
manganese root metal [Mn],x
technetium root metal [Tc],x
rhenium root metal [Re],x
iron root metal [Fe],x
ruthenium root metal [Ru],x
osmium root metal [Os],x
cobalt root metal [Co],x
rhodium root metal [Rh],x
iridium root metal [Ir],x
nickel root metal [Ni],x
palladium root metal [Pd],x
platinum root metal [Pt],x
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copper root metal [Cu],x
silver|argent root metal [Ag],x
gold root metal [Au],x
zinc root metal [Zn],x
cadmium root metal [Cd],x
mercury root metal [Hg],w
boron root nonmetal [B],x
aluminum|alane root metal [Al],x
gallium root metal [Ga],x
indium root metal [In],x
thallium root metal [Tl],x
carbon root nonmetal [C],x
silicon root nonmetal [Si],x
germanium root metal [Ge],x
tin root metal [Sn],x
lead root metal [Pb],x
nitrogen root nonmetal [N],x
phosphorus root nonmetal [P],x
arsenic root nonmetal [As],x
antimony|stibium root metal [Sb],x
bismuth root metal [Bi],x
oxygen root nonmetal [O],x
sulfur root nonmetal [S],x
selenium root nonmetal [Se],x
tellurium root nonmetal [Te],x
polonium nonroot metal [Po],x
fluorine root nonmetal [F],x
chlorine root nonmetal [Cl],x
bromine root nonmetal [Br],x
iodine root nonmetal [I],x
astatine root nonmetal [At],x
helium root nonmetal [He],x
neon root nonmetal [Ne],x
argon root nonmetal [Ar],x
krypton root nonmetal [Kr],x
xenon root nonmetal [Xe],x
radon root nonmetal [Rn],x

bromo|brom root root Br,4@x
iodo|iod root root I,4@x
iodosyl|iodoso root root I,4@x,=O,x
iodyl|iodoxy root root I,4@x,(=O)=O,x
deutero|deuterio root root [2H],4@x
nitro root root [N+],4@x,(=O)[O-],x
acinitro root root [N+],8@x,(O)[O-],x
nitroso|nitros|nitrosyl root root N=O,4@x
nitrosamido root root N,4@x,N=O,x
nitrosamide root root NN=O,x
nitrosonium root root [NH0+],x,=O,x
isonitroso|isonitros root root N,8@x,O,x
hydroxy|hydroxo root root O,4@x
hydroxyl root root O,4@o
hydroseleno root root [Se],4@x
hydrotelluro root root [Te],4@x
cyano|cyanogen root root C#N,4@x
isocyano|isonitrilo root root [N+]#[C-],4@x
cyanato root root OC#N,4@x
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isocyanato root root N=C=O,4@x
thiocyanato root root SC#N,4@x
isothiocyanato root root N=C=S,4@x
selenocyanato root root [Se]C#N,4@x
isoselenocyanato root root N=C=[Se],4@x
diazo root root [N+],8@x,=[N-],x
diazoate|diazoat root root [N+],8@x,=N,x,[O-],x
azido|triazo root root N,4@x,=[N+]=[N-],x
oxo|keto root root O,8@x
oxido root root [O-],4@x
thioxo|thiono root root S,8@x
sulfido root root [S-],4@x
selenoxo root root [Se],8@x
telluroxo root root [Te],8@x
mercapto root root S,4@x
hydroperoxy root root O,4@x,O,x
carboxy root root C,4@x,(=,x,O,x,),x,O,x
amidino root root C,4@x,(,x,N,x,)=,x,N,x
aminoiminometh root root C,x,(=,x,N,x,),x,N,x
sulfo root heterolover S,4@x,(=O),x,(=O),x,O,x
sulfoxy root root O,4@x,S,x,(=O),x,(=O),x,O,x
sulfoamido root root N,4@x,S,x,(=O),x,(=O),x,O,x
sulfino root root S,4@x,(=O),x,O,x
sulfeno root root S,4@x,O,x
sulfonato root root S,4@x,(=O),x,(=O),x,[O-],x
phosphonato|phosphato root root P,4@x,(=O),x,([O-]),x,[O-],x
hydrogenphosphato root root P,4@x,(=O),x,(O),x,[O-],x
dihydrogenphosphato root root P,4@x,(=O),x,(O),x,O,x
phosphinato root root P,4@x,(=O),x,[O-],x
phosphono|phosphoro infix infix P,4@x,(=O),x,(,x,O,1@o',),x,O,1@o
phospho root heterolover P,4@x,(=O),x,(O),1@x,O,1@x
diphospho root heterolover P,4@x,(=O),x,(O),1@x,O,x,P,x,(=O),x,(O),1@x,O,1@x
triphospho root heterolover
P,4@x,(=O),x,(O),1@x,O,x,P,x,(=O),x,(O),1@x,O,x,P,x,(=O),x,(O),1@x,O,1@x
phosphinico root root P,8@x,(=O),x,O,1@o
arsonato root root [As],4@x,(=O),x,([O-]),x,[O-],x
arsinato root root [As],4@x,(=O),x,[O-],x
arsono|arsoro root root [As],4@x,(=O),x,(,x,O,1@o',),x,O,1@o
arsinico root root [As],8@x,(=O),x,O,1@o
mesyl root root S,4@x,(=O),x,(=O),x,C,x
-part2-toluene root root C,4@a|alpha
-part2-cumene root root C,4@7|a|alpha,(,x,C,8|b|beta,),x,C,9
-part2-cymene root root C,4@8|a|alpha,(,x,C,9,),x,C,10
-part2-anisidine root root O,4@x,C,a|alpha
-part2-thioanisidine root root S,4@x,C,a|alpha
-part2-phenetidine root root O,4@x,C,a|alpha,C,b|beta
-part2-xylidine root root C,4@a|alpha
-part2-arsanil root root N,4@n
-part2-coumar root root O,4@x
indophenol root root
O,x,=,x,C,1,Ring,Ring1,C,2,=,x,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,=,x,N,x,C,
1',Ring,Ring2,=,x,C,2'|m|meta,C,3'|o|ortho,=,x,C,4',(,x,O,x,),x,C,5',=,x,C,6',Ri
ng,Ring2
thymolindophenol root root
O,x,=,x,C,1,Ring,Ring1,C,2,=,x,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,=,x,N,x,C,
1',Ring,Ring2,=,x,C,2'|m|meta,C,3'|o|ortho,(,x,C,x,(,x,C,x,),x,C,x,),x,=,x,C,4',
(,x,O,x,),x,C,5',=,x,C,6',(,x,C,x,),x,Ring,Ring2
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cresolindophenol root root
O,x,=,x,C,1,Ring,Ring1,C,2,=,x,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,=,x,N,x,C,
1',Ring,Ring2,=,x,C,2'|m|meta,(C),x,C,3'|o|ortho,=,x,C,4',(,x,O,x,),x,C,5',=,x,C
,6',Ring,Ring2
picoline|picolin|picol toluene picoline
c,2,Ring,Ring1,c,3|b|beta,c,4|g|gamma,c,5,c,6,n,1,Ring,Ring1
pipecoline|pipecolin|pipecol toluene picoline
C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,p,C,5,C,6,N,1,Ring,Ring1
toluene|tolu|tol toluene toluene
c,1,Ring,Ring1,c,2|o|ortho,Ring,Ring2,.,.,x,c,4|p|para,Ring,Ring3,Ring,Ring4,.,.,x,c
,6,Ring,Ring5,Ring,Ring1,.,.,x,c,3|m|meta,Ring,Ring2,Ring,Ring3,.,.,x,c,5,Ring,Ring4
,Ring,Ring5
toluidide|otoluidide|toluide|otoluide toluidide toluene
O,8@x,.,.,x,N,4@x,c,1',Ring,Ring1,c,2'|o|ortho,c,3'|m|meta,c,4'|p|para,c,5',c,6',R
ing,Ring1
cumidine|cumidin toluene cumene
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
cumene|cumen toluene cumene
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
cumyl|alphacumyl root root
C,4@a|alpha,(C)(C),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
cumidene|cumiden toluene cumene
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
cymene|cymen toluene cymene
C,7|a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylene|xylol toluene toluene
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylen|xyl toluene xylidine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylidide|oxylidide|xylide|oxylide toluidide xylidine
O,8@x,.,.,x,N,4@x,c,1',Ring,Ring1,c,2'|o|ortho,c,3'|m|meta,c,4'|p|para,c,5',c,6',R
ing,Ring1
anis toluene anisidine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
thioanis toluene thioanisidine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
homoanis toluene anisidine
C,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anisidide|oanisidide|aniside|oaniside toluidide anisidine
O,8@x,.,.,x,N,4@x,c,1',Ring,Ring1,c,2'|o|ortho,c,3'|m|meta,c,4'|p|para,c,5',c,6',R
ing,Ring1
anisal toluene anisidine
C,8@x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
mentha|menth|neomenth|neomentha|isomenth|isomentha toluene cymene
C,3|m|meta,Ring,Ring1,C,4|p|para,C,5,C,6,C,1,Ring,Ring2,C,2|o|ortho,Ring,Ring1,.
,x,C,7|a|alpha,Ring,Ring2
anisidine|anisidin toluene anisidine
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anisidino toluene anisidine
N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
phenetidine|phenetidin toluene phenetidine
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
phenetidide|ophenetidide|phenetide|ophenetide toluidide phenetidine
O,8@x,.,.,x,N,4@x,c,1',Ring,Ring1,c,2'|o|ortho,c,3'|m|meta,c,4'|p|para,c,5',c,6',R
ing,Ring1
phenetidino toluene phenetidine
N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1

cresyl toluene toluene
O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
cres toluene toluene
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
thiocresol toluene toluene
S,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
cresylicacid toluene toluene
O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
cresot toluene toluene
c,2,Ring,Ring1,(O),x,c,3|o|ortho,c,4|m|meta,c,5|p|para,c,6,c,1,(,x,C,x,),x,Ring,
Ring1
toluidine|toluidin toluene toluene
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
toluidino toluene toluene
N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylidine|xylidin toluene xylidine
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylidino toluene xylidine
N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
coumar toluene coumar
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c,6,Ring,Ring1
arsanil toluene tolarsanil
[As],x,(,x,O,1@x,),x,(,x,O,1@x,),x,(=O),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,
c,4|p|para,c,5,c,6,Ring,Ring1
tosyl|ptosyl root root
S,4@x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc,x,(,x,C,x,),x,cc,x,Ring,Ring1
tosylate|ptosylate|tosylat|ptosylat|tosilate|ptosilate|tosilat|ptosilat root
root O,1@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(C)cc,x,Ring,Ring1
tosylamido root root
N,4@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(C)cc,x,Ring,Ring1
brosylate|brosylat|brosilate|brosilat root root
O,1@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(Br)cc,x,Ring,Ring1
brosyl root root S,4@x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(Br)cc,x,Ring,Ring1
closylate|closylat|closilate|closilat root root
O,1@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(Cl)cc,x,Ring,Ring1
closyl root root S,4@x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(Cl)cc,x,Ring,Ring1
nosylate|nosylat|nosilate|nosilat root root
O,1@x,S,x,(=O),x,(=O),x,c,x,Ring,Ring1,cc([N+](=O)[O-])ccc,x,Ring,Ring1
mesylate|mesylat root root O,1@x,S,x,(=O),x,(=O),x,C,x
esylate|esylat root root O,1@x,S,x,(=O),x,(=O),x,C,x,C,x
pipsyl root root S,4@x,(=O),x,(=O),x,c,x,Ring,Ring1,ccc(I)cc,x,Ring,Ring1
methosulfate|methosulfat|metilsulfate|metilsulfat root root
O,1@x,S,x,(=O),x,(=O),x,O,x,C,x
ethosulfate|ethosulfat|etilsulfate|etilsulfat root root
O,1@x,S,x,(=O),x,(=O),x,O,x,C,x,C,x
desyl root root C,x,(C(=O)c1ccccc1)c2ccccc2,x
isoniazide|isoniazid root root
c,2,Ring,Ring1,c,3,c,4,(,x,C,x,(,x,=,x,O,x,),x,N,x,N,n,),x,c,5,c,6,n,1,Ring,Ring
1
pheneth root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring
,Ring1
secpheneth root root
C,a|alpha,(,x,C,b|beta,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c,6,Ring,Ring1

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neoph root root
C,a|alpha,C,b|beta,(C)(C),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5
,c,6,Ring,Ring1
amphetamine|amphetamin root root
N,n,C,a|alpha,(C),x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,
5,c,6,Ring,Ring1
methamphetamine|methamphetamin root root
C,x,N,n,C,a|alpha,(C),x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|par
a,c,5,c,6,Ring,Ring1
ammelide root root
N,n,c,6,Ring,Ring1,n,1,c,2,(,x,O,x,),x,n,3,c,4,(,x,O,x,),x,n,5,Ring,Ring1
phenate|phenat|phenoxide|phenoxid root root [O-
],x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
phen root phenyl
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
benzyne|benzyn root root
C,1,Ring,Ring1,#,x,C,2|o|ortho,C,3|m|meta,=,x,C,4|p|para,C,5,=,x,C,6,Ring,Ring1
benzal root root
C,8@a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
benzene|benzen|benzol root root
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
dewarbenzene root root C12C=CC1C=C2,x
benzeneoxid|benzeneoxide root root
C,1,Ring,Ring1,(,x,O,x,Ring,Ring2,),x,C,2,Ring,Ring2,C,3,=,x,C,4,C,5,=,x,C,6,Rin
g,Ring1
benzo-quinone|benzo-quinon root root
C,1,Ring,Ring1,(=O),x,C,2|o|ortho,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x,C,6,R
ing,Ring1
benzo-quinodimethane|benzo-quinodimethan root root
C,1,Ring,Ring1,(=,x,C,2@7,),x,C,2|o|ortho,=,x,C,3|m|meta,C,4|p|para,(=,x,C,2@8,)
,x,C,5,=,x,C,6,Ring,Ring1
toluquinone|ptoluquinone root root
C,1,Ring,Ring1,(=O),x,C,2|o|ortho,(C),x,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x
,C,6,Ring,Ring1
xyloquinone|pxyloquinone root root
C,1,Ring,Ring1,(=O),x,C,2|o|ortho,(C),x,=,x,C,3|m|meta,C,4|p|para,(=O),x,C,5,=,x
,C,6,(C),x,Ring,Ring1
duroquinone root root CC(C(C(C)=C1C)=O)=C(C1=O)C,x
thymoquinone root root O=C(C(C)=C1)C=C(C1=O)C(C)C,x
hemellitol root root
c,1,(C),x,Ring,Ring1,c,2|o|ortho,(C),x,c,3|m|meta,(C),x,c,4|p|para,c,5,c,6,Ring,
Ring1
benzo|benz benzo benzo
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
acene|acen acene acene c1ccccc1,x
aphene acene aphene c1ccccc1,x
mandel|amygdal root root
C,x,C,x,(,x,O,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Rin
g,Ring1
mesit root root
c,2|o|ortho,Ring,Ring1,c,3|m|meta,(,x,C,alpha1|alpha2|alpha,),x,c,4|p|para,c,5,(
,x,C,alpha3|alpha4|alpha',),x,c,6,c,1,(,x,C,alpha5|alpha6|alpha'',),x,Ring,Ring1
mesitylene|mesitylen root root
C,alpha1|alpha2|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,C,alpha3|alpha4|
alpha',),x,c,4|p|para,c,5,(,x,C,alpha5|alpha6|alpha'',),x,c,6,Ring,Ring1
durene|duren root root
C,a|alpha|alpha1,c,1,Ring,Ring1,c,2|o|ortho,(,x,C,a'|alpha'|alpha2,),x,c,3|m|met

a,c,4|p|para,(,x,C,a''|alpha''|alpha4,),x,c,5,(,x,C,a'''|alpha'''|alpha5,),x,c,6
,Ring,Ring1
isodurene|isoduren root root
C,a|alpha|alpha1,c,1,Ring,Ring1,c,2|o|ortho,(,x,C,a'|alpha'|alpha2,),x,c,3|m|met
a,(,x,C,a''|alpha''|alpha3,),x,c,4|p|para,c,5,(,x,C,a'''|alpha'''|alpha5,),x,c,6
,Ring,Ring1
anisole|anisol root root
C,a|alpha,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring
1
catechol root root
c,1,Ring,Ring1,(,x,O,o,),x,c,2|ortho,(,x,O,o',),x,c,3|m|meta,c,4|p|para,c,5,c,6,
Ring,Ring1
phenetole|phenetol root root
C,b|beta,C,a|alpha,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,
Ring,Ring1
anethole|anethol root root
C,x,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(,x,C,x,=,x,C,x,C,x,),x
,c,5,c,6,Ring,Ring1
dihydroanethole|dihydroanethol root root
C,x,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,C,x,),x,c,5
,c,6,Ring,Ring1
guaiacol root root
C,x,O,x,c,2|o|ortho,Ring,Ring1,c,1,(,x,O,x,),x,c,6,c,5,c,4|p|para,c,3|m|meta,Rin
g,Ring1
guaiacolate root root
C,x,O,x,c,2|o|ortho,Ring,Ring1,c,1,(,x,O,1@x,),x,c,6,c,5,c,4|p|para,c,3|m|meta,R
ing,Ring1
veratrole|veratrol root root
C,x,O,x,c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,c,5,c,6
,Ring,Ring1
eugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,=,x
,C,x,),x,c,5,c,6,Ring,Ring1
dihydroeugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,C,x
,),x,c,5,c,6,Ring,Ring1
isoeugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,=,x,C,x
,C,x,),x,c,5,c,6,Ring,Ring1
isoeugenol root root
O,x,c,1,Ring,Ring1,c,2|o|ortho,(,x,O,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,=,x
,C,x,C,x,),x,c,5,c,6,Ring,Ring1
styr|styrene|styren|styrol|cinnamene|cinnamenol|cinnamol root root
C,b|beta|w|omega,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,
c,5,c,6,Ring,Ring1
styrall|styral root root
C,b|beta,(,x,C,a|alpha,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c,6,Ring,Ring1
phosphinine root root
p,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anthranil root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,(,x,N,n,),x,c,3|m|meta,c,4|p|para,c,5,c,6,R
ing,Ring1
hippur root trivial
C,x,C,x,N,x,C,x,(,x,=,x,O,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para
,c,5,c,6,Ring,Ring1

carbanil loveracid root
C,x,N,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
shikim root root
C,x,C,1,Ring,Ring1,=,x,C,2,C,3,(O),x,C,4,(O),x,C,5,(O),x,C,6,Ring,Ring1
benzo|benz|dracyl root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
crithmin root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(C),x,c,5,c,6,Ring,Ri
ng1
dracon root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(OC),x,c,5,c,6,Ring,R
ing1
vanill root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,),x,c,4|p|para,(,x,O
,x,),x,c,5,c,6,Ring,Ring1
isovanill root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(O),x,c,4|p|para,(OC),x,c,5,c,6,
Ring,Ring1
homovanill root root
C,a|alpha,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,),x,c,4|p|para,(
,x,O,x,),x,c,5,c,6,Ring,Ring1
vanillin root root
O,x,Ring,Ring2,.,x,O,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),
x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
ethylvanillin root root
O,x,Ring,Ring2,.,x,O,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OCC)
,x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
isovanillin root root
O,x,Ring,Ring2,.,x,O,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,Ring,
Ring2,c,4|p|para,(OC),x,c,5,c,6,Ring,Ring1
acetovanillone root root
O,x,=,x,C,a|alpha,(C),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,),x,c,
4|p|para,(,x,O,x,),x,c,5,c,6,Ring,Ring1
safrole|safrol root root
C,x,=,x,C,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2
,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
dihydrosafrole|dihydrosafrol root root
C,x,C,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2,),x
,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
isosafrole|isosafrol root root
C,x,C,x,=,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2
,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
piperon root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ring2,),x,c
,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
homopiperon root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,C,x,O,x,Ring,Ri
ng2,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
veratr root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|para,(OC),x,c,5,c,6
,Ring,Ring1
homoveratr root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|para,(OC),
x,c,5,c,6,Ring,Ring1
protocatechu root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,),x,c,4|p|para,(,x,O,x,)
,x,c,5,c,6,Ring,Ring1

homoprotocatechu root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,),x,c,4|p|para,
(,x,O,x,),x,c,5,c,6,Ring,Ring1
citrazin root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,),x,n,4|p|para,c,5,(,x,O
,x,),x,c,6,Ring,Ring1
gall root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,O,x,),x,c,4|p|para,(,x,O,x,)
,x,c,5,(,x,O,x,),x,c,6,Ring,Ring1
gallacetophenone root root O=C(C)C1=C(O)C(O)=C(O)C=C1,x
toluene|toluol root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring
1
cumene|cumen root root
C,x,C,a|alpha,(,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c
,6,Ring,Ring1
aniline|anilin|analine|analin root root
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anilino|analino root root
N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
gentis root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,(,x,O,o',),x,c,6,Ri
ng,Ring1
homogentis root root
C,x,C,x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,(,x,O,o',),x,c,
6,Ring,Ring1
salicyl|salic root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
salicylal root root
C,8@x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anilot root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,o,),x,c,3|m|meta,c,4|p|para,c,5,([N+](=O)[O-
]),x,c,6,Ring,Ring1
alpharesorcyl|aresorcyl root root
C,x,c,1,Ring,Ring1,c,2,c,3|m|meta,(,x,O,x,),x,c,4|p|para,c,5,(,x,O,x,),x,c,6,Rin
g,Ring1
betaresorcyl|bresorcyl root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,x,),x,c,3|m|meta,c,4|p|para,(,x,O,x,),x,c,5,c,6,Rin
g,Ring1
gammaresorcyl|gresorcyl root root
C,x,c,1,Ring,Ring1,c,2,(,x,O,x,),x,c,3|m|meta,c,4|p|para,c,5,c,6,(,x,O,x,),x,Rin
g,Ring1
phenac root root
C,a|alpha,C,x,(,x,=,x,O,x,),x,c,x,Ring,Ring1,=,x,c,2|o|ortho,c,3|m|meta,c,4|p|pa
ra,c,5,c,6,Ring,Ring1
trop root root
C,x,C,x,(,x,C,x,O,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6
,Ring,Ring1
nortrop root root
C,x,(,x,C,x,O,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Rin
g,Ring1
hydratrop root root
C,x,C,x,(,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Rin
g,Ring1
homatrop root root CN1C2CCC1CC(OC(C(O)C3=CC=CC=C3)=O)C2,x
atrop root root OCC(C(OC3CC2CCC(C3)N2C)=O)c1ccccc1,x

tropan|tropane root root C,3,(,x,C,2,C,1,Ring,Ring1,Ring,Ring2,),x,C,4,C,5|a-
r,(,x,C,6|a-b,C,7|a-t,Ring,Ring2,),x,N,8,Ring,Ring1,C,x
tropin|tropine root root C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,(O),x,C,4,C,5|a-
r,(,x,C,6|a-b,C,7|a-t,Ring,Ring2,),x,N,8,Ring,Ring1,C,x
1alphah5alphahtropan root root
C,3,(,x,C,2,[C@],1,([H]),x,Ring,Ring1,Ring,Ring2,),x,C,4,[C@],5|a-
r,([H]),x,(,x,C,6|a-b,C,7|a-t,Ring,Ring2,),x,N,8,Ring,Ring1,C,x
tropinone root root CN1C(C2)CCC1CC2=O,x
atrolact root root
C,x,C(C)(O),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring
1
cinnamo|cinnam root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c,6,Ring,Ring1
cinnamal root root
C,8@x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,
5,c,6,Ring,Ring1
hydrocinnam root root
C,x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,
Ring,Ring1
hydrocinnamal root root
C,8@x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,
6,Ring,Ring1
grevill root root
C,x,/,x,C,a|alpha,=,x,C,b|beta,/,x,c,1,Ring,Ring1,c,2|o|ortho,(O),x,c,3|m|meta,c
,4|p|para,c,5,(O),x,c,6,Ring,Ring1
caffe root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(O),x,c,4|p|par
a,(O),x,c,5,c,6,Ring,Ring1
ferul root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
ra,(O),x,c,5,c,6,Ring,Ring1
sinap root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
ra,(O),x,c,5,(OC),x,c,6,Ring,Ring1
conifer|conifero root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
ra,(O),x,c,5,c,6,Ring,Ring1
phloret root root
C,x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(O),x,c,
5,c,6,Ring,Ring1
nicotino|nicotine|nicotin loveracid root
C,x,c,3,Ring,Ring1,c,4,c,5,c,6,n,1,c,2,Ring,Ring1
nicotin root root C,x,c,3,Ring,Ring1,c,4,c,5,c,6,n,1,c,2,Ring,Ring1
isonicotino|isonicotin root root
c,x,c,4,Ring,Ring1,c,5,c,6,n,1,c,2|a|alpha,c,3|b|beta,Ring,Ring1
melamine|melamin root root
n,1,Ring,Ring1,c,2,(N),x,n,3,c,4,(N),x,n,5,c,6,(N),x,Ring,Ring1
pyrylium root root
[o+],1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
naphtho|naphth|naphthalene|naphthalen root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a|4alpha,Ring,Ring2,c,5,c,6,c,7,c,8
,c,8a|8alpha,Ring,Ring1,Ring,Ring2
naphtho|naphth opfuser unknown
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a|4alpha,Ring,Ring2,c,5,c,6,c,7,c,8
,c,8a|8alpha,Ring,Ring1,Ring,Ring2

naphtho-quinone|naphtho-quinon|naphthalene-quinone|naphthalene-quinon root root
c,1|a|alpha,(=O),x,Ring,Ring1,c,2|b|beta,=,x,c,3,c,4,(=O),x,c,4a|4alpha,Ring,Rin
g2,c,5,c,6,c,7,c,8,c,8a|8alpha,Ring,Ring1,Ring,Ring2
cadalene|cadalen root root
c,1|a|alpha,(C),x,Ring,Ring1,c,2|b|beta,c,3,c,4,(C(C)C),x,c,4a|4alpha,Ring,Ring2
,c,5,c,6,(C),x,c,7,c,8,c,8a|8alpha,Ring,Ring1,Ring,Ring2
benzodioxene|benzodioxen root root
o,1,Ring,Ring1,c,2,c,3,o,4,c,4a|4alpha,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a|8alpha,Ri
ng,Ring1,Ring,Ring2
azulene|azulen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
Ring2
azuleno|azulen opfuser unknown
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
Ring2
anthracene|anthracen|anthro|anthr root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,10,c,5a|10a,Ring,Rin
g3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
anthrone|anthron root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,C,10,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,C,9,(=,x,O,x,),x,c,9a,Ring,Ring2,Ring,Ring1
anthra-quinone|anthra-quinon|anthracene-quinone|anthracene-quinon root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,C,10,(=O),x,c,5a|10a,R
ing,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,C,9,(=,x,O,x,),x,c,9a,Ring,Ring2,Ring,
Ring1
anthra|anthraceno opfuser unknown
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,10,c,5a|10a,Ring,Rin
g3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
acrid root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,n,10,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
aminacrine|aminacrin|aminacridin|aminacridine|monacrin|monacrine root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,n,10,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,(N),n,c,9a,Ring,Ring2,Ring,Ring1
acenaphthene|acenaphthen root root
C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring,Ring1,c,8b,Ring,Ring2,Ring,Ring3
acenaphtho|acenaphth opfuser unknown
C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring,Ring1,c,8b,Ring,Ring2,Ring,Ring3
acenaphthylene|acenaphthylen root root
c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring,Ring1,c,8b,Ring,Ring2,Ring,Ring3
cholanthrene|cholanthren root root
C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
g4,c,6b,Ring,Ring5,c,7,c,8,c,9,c,10,c,10a,Ring,Ring5,c,11,c,12,c,12a,Ring,Ring4,
c,12b,Ring,Ring1,c,12c,Ring,Ring3,Ring,Ring2
phenalene|phenalen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
,9a,Ring,Ring1,c,9b,Ring,Ring2,Ring,Ring3
julolid root root
C,1,Ring,Ring1,C,2,c,C,N,4,Ring,Ring2,C,5,C,6,C,7,c,7a,Ring,Ring3,c,8,c,9,c,10,c
,10a,Ring,Ring1,c,10b,Ring,Ring2,Ring,Ring3
perimid root root
n,1,Ring,Ring1,c,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
,9a,Ring,Ring1,c,9b,Ring,Ring2,Ring,Ring3

phenanthren|phenanthrene root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring,Ring3,c,9,c,10,c,10a,Ring,Ring1,Ring,Ring2
phenanthr|phenanthro|phenanthra opfuser unknown
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring,Ring3,c,9,c,10,c,10a,Ring,Ring1,Ring,Ring2
cyclopentadefphenanthren|cyclopentadefphenanthrene root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,4a,Ring,Ring3,c,5,c,6,c,7,c,7a,Ring
,Ring4,c,8,c,9,c,8a,Ring,Ring1,c,8b,Ring,Ring2,c,8c,Ring,Ring3,Ring,Ring4
bathophenanthroline root root
n,1,Ring,Ring1,c,2,c,3,c,4,(c4ccccc4),x,c,4a,Ring,Ring2,c,5,c,6,c,6a,Ring,Ring3,
c,7,(c5ccccc5),x,c,8,c,9,n,10,c,10a,Ring,Ring3,c,10b,Ring,Ring1,Ring,Ring2
phenanthrone|phenanthron root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring,Ring3,C,9,(=O),x,C,10,c,10a,Ring,Ring1,Ring,Ring2
phenanthrene-quinone|phenanthrene-quinon root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring,Ring3,c,9,(=O),x,c,10,(=O),x,c,10a,Ring,Ring1,Ring,Ring2
cyclopentaaphenanthrene|cyclopentaaphenanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring2,c,6,c,7,c,8,Ring,Ring3,c,14,Ring,Ring4
,c,15,c,16,c,17,c,13,Ring,Ring4,c,12,c,11,c,9,Ring,Ring3,c,10,Ring,Ring2,Ring,Ri
ng1
fluoranthene|fluoranth|fluoranthen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
3
acephenanthrene|acephenanthren root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,ring2,C,4,C,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
3
acephenanthrylene|acephenanthrylen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
3
aceanthrene|aceanthren root root
C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
3
aceanthrylene|aceanthrylen root root
c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
3
violanthrene|violanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,C,5,c,5a,Ring,Ring3,c,6,c,7,c,7a,Ring
,Ring4,c,7b,Ring,Ring5,c,8,c,9,c,9a,(,x,c,18f,Ring,Ring6,c,18e,Ring,Ring7,Ring,R
ing5,),x,C,10,c,10a,Ring,Ring8,c,11,c,12,c,13,c,14,c,14a,Ring,Ring8,c,14b,Ring,R
ing6,c,15,c,16,c,16a,Ring,Ring7,c,16b,Ring,Ring9,c,17,c,18,c,18a,(,x,c,18b,Ring,
Ring1,Ring,Ring2,),x,c,18c,Ring,Ring3,c,18d,Ring,Ring4,Ring,Ring9
isoviolanthrene|isoviolanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,6a,(,x,c,18
c,Ring,Ring4,c,18b,Ring,Ring5,Ring,Ring3,),x,c,6b,Ring,Ring6,c,7,c,8,c,8a,(,x,c,
18e,Ring,Ring7,c,18d,Ring,Ring8,Ring,Ring6,),x,C,9,c,9a,Ring,Ring9,c,10,c,11,c,1
2,c,13,c,13a,Ring,Ring9,c,13b,Ring,Ring7,c,14,c,15,c,15a,Ring,Ring8,c,15b,Ring,R
ing4,c,16,c,17,c,17a,Ring,Ring5,C,18,c,18a,Ring,Ring1,Ring,Ring2
triphenylene|triphenylen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,

Ring,Ring3,c,8b,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,c,12b,Ring,Ring2,
Ring,Ring1
trindene|trinden root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,3b,Ring,Ring3,c,4,c,5,c,6,c,6a,Ring,Rin
g3,c,6b,Ring,Ring4,c,7,c,8,c,9,c,9a,Ring,Ring4,c,9b,Ring,Ring2,Ring,Ring1
pyrene|pyren root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring,Ring4,c,9,c,10,c,10a,Ring,Ring1,c,10b,Ring,Ring2,c,10c,Ring,Ring3,Ring,Ring
4
chrysene|chrysen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,6a,Ring,Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring3,c,11,c,12,c,12a,Ring,Ring2
,Ring,Ring1
naphthacene|naphthacen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,11,c,11a,Ring,Ring3,c,12,c,12a,Ring,Ring2
,Ring,Ring1
naphthaceno|naphthacen opfuser unknown
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,11,c,11a,Ring,Ring3,c,12,c,12a,Ring,Ring2
,Ring,Ring1
pleiadene|pleiaden root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,7a,Ring
,Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,12,c,12a,Ring,Ring1,c,12b,Ring,Ring3
,Ring,Ring2
picene|picen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Rin
g4,c,7,c,8,c,8a,Ring,Ring5,c,9,c,10,c,11,c,12,c,12a,Ring,Ring5,c,12b,Ring,Ring4,
c,13,c,14,c,14a,Ring,Ring3,c,14b,Ring,Ring2,Ring,Ring1
perylene|perylen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Rin
g4,c,7,c,8,c,9,c,9a,Ring,Ring5,c,10,c,11,c,12,c,12a,(,x,c,12d,Ring,Ring5,Ring,Ri
ng4,),x,c,12b,Ring,Ring1,c,12c,Ring,Ring2,Ring,Ring3
perylo opfuser unknown
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Rin
g4,c,7,c,8,c,9,c,9a,Ring,Ring5,c,10,c,11,c,12,c,12a,(,x,c,12d,Ring,Ring5,Ring,Ri
ng4,),x,c,12b,Ring,Ring1,c,12c,Ring,Ring2,Ring,Ring3
tetraphenylene|tetraphenylen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring,Ring3,c,8b,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,c,12b,Ring,Ring5,
c,13,c,14,c,15,c,16,c,16a,Ring,Ring5,c,16b,Ring,Ring2,Ring,Ring1
rubicene|rubicen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,3b,Ring,Ring3,c,4,c,5,c,6,c,7,c,7a,Ring
,Ring3,c,7b,Ring,Ring4,c,7c,Ring,Ring5,c,8,c,9,c,10,c,10a,Ring,Ring6,c,10b,Ring,
Ring7,c,11,c,12,c,13,c,14,c,14a,Ring,Ring7,c,14b,(,x,c,14e,Ring,Ring6,Ring,Ring5
,),x,c,14c,Ring,Ring1,c,14d,Ring,Ring2,Ring,Ring4
coronene|coronen root root
c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,4a,Ring,Ring3,c,5,c,6,c,6a,Ring,Rin
g4,c,7,c,8,c,8a,Ring,Ring5,c,9,c,10,c,10a,Ring,Ring6,c,11,c,12,c,12a,Ring,Ring1,
c,12b,Ring,Ring7,c,12c,Ring,Ring2,c,12d,Ring,Ring3,c,12e,Ring,Ring4,c,12f,Ring,R
ing5,c,12g,Ring,Ring6,Ring,Ring7
trinaphthylene|trinaphthylen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,5b,Ring,Ring4,c
,6,c,6a,Ring,Ring5,c,7,c,8,c,9,c,10,c,10a,Ring,Ring5,c,11,c,11a,Ring,Ring4,c,11b
,Ring,Ring6,c,12,c,12a,Ring,Ring7,c,13,c,14,c,15,c,16,c,16a,Ring,Ring7,c,17,c,17
a,Ring,Ring6,c,17b,Ring,Ring3,c,18,c,18a,Ring,Ring2,Ring,Ring1

pyranthrene|pyranthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,5a,Ring,Ring4,c
,6,c,7,c,7a,Ring,Ring5,c,8,c,8a,Ring,Ring6,c,9,c,10,c,11,c,12,c,12a,Ring,Ring6,c
,12b,Ring,Ring7,c,13,c,13a,Ring,Ring8,c,14,c,15,c,15a,(,x,c,16,c,16a,Ring,Ring2,
Ring,Ring1,),x,c,15b,Ring,Ring3,c,15c,Ring,Ring8,c,15d,Ring,Ring4,c,15e,Ring,Rin
g7,Ring,Ring5
ovalene|ovalen root root
c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,4a,Ring,Ring3,c,5,c,6,c,6a,Ring,Rin
g4,c,7,c,7a,Ring,Ring5,c,8,c,9,c,9a,Ring,Ring6,c,10,c,11,c,11a,Ring,Ring7,c,12,c
,13,c,13a,Ring,Ring8,c,14,c,14a,Ring,Ring1,c,14b,Ring,Ring9,c,14c,Ring,Ring2,c,1
4d,Ring,Ring3,c,14e,Ring,Ring4,c,14f,Ring,Ring0,c,14g,Ring,Ring5,c,14h,Ring,Ring
6,c,14i,Ring,Ring7,c,14j,Ring,Ring8,c,14k,Ring,Ring0,Ring,Ring9
biphenylene|biphenylen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring,Ring3,c,8b,Ring,Ring2,Ring,Ring1
thianthrene|thianthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,s,10,c,10a,Ring,Ring2,Ring,Ring1
pyr root root
c,2|a|alpha,Ring,Ring1,c,3|b|beta,c,4|g|gamma,c,5,c,6,o,1,Ring,Ring1
pyrano opfuser unknown c,2,Ring,Ring1,c,3,c,4,c,5,c,6,o,1,Ring,Ring1
mdioxine|mdioxin root root c,2,Ring,Ring1,o,3,c,4,c,5,c,6,o,1,Ring,Ring1
pdioxine|pdioxin root root c,2,Ring,Ring1,c,3,o,4,c,5,c,6,o,1,Ring,Ring1
oxalene|oxalen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,o,7,c,7a,Ring,Ring2,Ring,Ring
1
azalene|azalen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,n,7,c,7a,Ring,Ring2,Ring,Ring
1
isobenzofuran root root
c,1,Ring,Ring1,o,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ring,Ring
1
benzofurazan root root
n,1,Ring,Ring1,o,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ring,Ring
1
benzofuroxan root root [n+],1,(,x,[O-
],x,),x,Ring,Ring1,o,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ring,
Ring1
piazthiole root root
n,1,Ring,Ring1,s,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ring,Ring
1
catecholborane root root
o,x,Ring,Ring1,B,b,O,x,c,2,Ring,Ring2,c,3,c,4,c,5,c,6,c,1,Ring,Ring2,Ring,Ring1
chromene|chromen root root
c,2,Ring,Ring1,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,1,Ring,
Ring1
chromane|chroman root root
C,2,Ring,Ring1,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,O,1,Ring,
Ring1
chromone|chromon root root
c,2,Ring,Ring1,c,3,c,4,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,
1,Ring,Ring1
esculetin root root
c,2,Ring,Ring1,(=O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,(O),x,c,7,(O),x,c,8,c,8a,R
ing,Ring2,o,1,Ring,Ring1

umbelliferone root root
c,2,Ring,Ring1,(=O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ri
ng2,o,1,Ring,Ring1
umbelliferyl root root
c,2,Ring,Ring1,(=O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,4@7,c,8,c,8a,Ring,Ring2,
o,1,Ring,Ring1
isochromane|isochroman root root
C,1,Ring,Ring1,O,2,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
Ring2
flav root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,C,4|a-
1,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,O,1,Ring,Ring1,),x,c,1',Ring,R
ing3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
flavone|flavon root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x,c,1'
,Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
acacetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(OC),x,c,5',c,6',Ring,Ring3
alpinetin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(OC),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,R
ing1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
apigenin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
baicalein root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(O),x,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,R
ing,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
catechin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,(O),x,C,4|a-
1,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,O,1,Ring,Ring1,),x
,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
chrysin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3
cirsiliol root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(OC),x,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1
,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
diosmetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
epicatechin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,(O),x,C,4|a-
1,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x
,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
eupatorin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,(OC),x,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1
,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
galangin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
genkwanin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1,Ring,R
ing1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
hesperitin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(OC),x,c,5',c,6',Ring,Ring3
kaempferide|kaempferol root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3

luteolin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
morin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',(O),x,c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
myricetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',(O),x,c,6',Ring,Ring3
naringenin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
pinocembrin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
pinostrobin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1,Ring,R
ing1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
quercetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3
robinetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),
x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',(O),x,c,6',Ring,Ring3
sinensetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(OC),x,c,6,(OC),x,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,
1,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(OC),x,c,5',c,6',Ring,Rin
g3
syringetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3
tectochrysin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring2,o,1,Ring,R
ing1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
isoflavone|isoflavon root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x,c,1'
,Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
daidzein root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),
x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
formononetin root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),
x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
genistein root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-
1,(=O),x,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring3
flavylium root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,),x,c,1',Rin
g,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
malvidin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,
),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3
cyanidin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(O),x,c,4|a-
1,c,4a,Ring,Ring2,c,5,(O),x,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,
),x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(O),x,c,5',c,6',Ring,Ring3

flavanone|flavanon root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,C,4|a-
l,(=O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,O,1,Ring,Ring1,),x,c,1'
,Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
anaphthoflavone|anaphthoflavon|alphanaphthoflavone|alphanaphthoflavon root root
O=C2C=C(C4=CC=CC=C4)OC1=C3C(C=CC=C3)=CC=C12,x
bnaphthoflavone|bnaphthoflavon|betanaphthoflavone|betanaphthoflavon root root
O=C2C=C(C3=CC=CC=C3)OC1=CC=C4C(C=CC=C4)=C12,x
xanthene|xanthen|xanthydr|xanth root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,10,c,10a,Ring,R
ing3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
xanthone|xanthon root root
c,9,Ring,Ring1,(,x,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,10,c,10a,Ri
ng,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1,),x,=O,x
xanthylium root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,[o+],10,c,10a,Rin
g,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
xanthuren root root
C,x,c,2,Ring,Ring1,c,3,c,4,(O),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,(O),x,c,8a,Ring
,Ring2,n,1,Ring,Ring1
thioxanthene|thioxanthen root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,10,c,10a,Ring,R
ing3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
selenoxanthene|selenoxanthen root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,[se],10,c,10a,Rin
g,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
acridars root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,c,10,c,10a,Ring,Ring2,Ring,Ring1
arsanthrene|arsanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
phosphanthrene|phosphanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,p,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,p,10,c,10a,Ring,Ring2,Ring,Ring1
selenanthrene|selenanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[se],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,[se],10,c,10a,Ring,Ring2,Ring,Ring1
phenomercurin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[Hg],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,[Hg],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxathiin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,s,10,c,10a,Ring,Ring2,Ring,Ring1
phenoxastannin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Sn],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxasilin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Si],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxagermanin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Ge],10,c,10a,Ring,Ring2,Ring,Ring1
phenothiastannin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,S,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Sn],10,c,10a,Ring,Ring2,Ring,Ring1

phenothiasilin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,S,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Si],10,c,10a,Ring,Ring2,Ring,Ring1
phenothiagermanin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,S,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Ge],10,c,10a,Ring,Ring2,Ring,Ring1
phenaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,n,10,c,10a,Ring,Ring2,Ring,Ring1
phenazasiline|phenazasilin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,N,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Si],10,c,10a,Ring,Ring2,Ring,Ring1
phenarsaz|phenoarsaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
phenothiaz|thiodiphenylamine root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,n,10,c,10a,Ring,Ring2,Ring,Ring1
phenomercaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,N,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Hg],10,c,10a,Ring,Ring2,Ring,Ring1
phenophosphaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,p,10,c,10a,Ring,Ring2,Ring,Ring1
phenotelluraz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[Te],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,N,10,c,10a,Ring,Ring2,Ring,Ring1
phenoselenaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[Se],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,N,10,c,10a,Ring,Ring2,Ring,Ring1
phenothiars root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxantimon root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Sb],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxars root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxaphos root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,P,10,c,10a,Ring,Ring2,Ring,Ring1
phenoxatellur root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Te],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxaselen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Se],10,c,10a,Ring,Ring2,Ring,Ring1
dibenzodioxin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,o,10,c,10a,Ring,Ring2,Ring,Ring1
phenoxaz|phenazox root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,n,10,c,10a,Ring,Ring2,Ring,Ring1
indene|inden root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2

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indeno opfuser unknown
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
indole|indol root root
n,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1,Ring,Ring2
thianaphthene|thianaphthen|thionaphthene|thionaphthen root root
s,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1,Ring,Ring2
thianaphtheno|thianaphthen opfuser unknown
s,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1,Ring,Ring2
isothianaphthene|isothianaphthen root root
c,1,Ring,Ring1,s,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1,Ring,Ring2
isothianaphtheno|isothianaphthen opfuser unknown
c,1,Ring,Ring1,s,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1,Ring,Ring2
skatole|skatol root root
n,1,Ring,Ring1,c,2,c,3,(C),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Rin
g,Ring2
gramine root root
n,1,Ring,Ring1,c,2,c,3,(CN(C)C),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
1,Ring,Ring2
indolo opfuser unknown
n,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
isoindole|isoindol root root
c,1,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
isoindolo opfuser unknown
c,1,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
arsindole|arsindol root root
[as],1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,R
ing2
arsindolo opfuser unknown
[as],1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,R
ing2
isoarsindole|isoarsindol root root
c,1,Ring,Ring1,[as],2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,R
ing2
isoarsindolo|isoarsindol opfuser unknown
c,1,Ring,Ring1,[as],2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,R
ing2
phosphindole|arsindol root root
p,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
phosphindolo|arsindol opfuser unknown
p,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
isophosphindole|isoarsindol root root
c,1,Ring,Ring1,p,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
isophosphindolo|isoarsindol opfuser unknown
c,1,Ring,Ring1,p,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2

indazole|indazol root root

n,1,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2

indazolo|indazol opfuser unknown

n,1,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2

indolizine|indolizin|pyrrocol root root

c,1,Ring,Ring1,c,2,c,3,n,4,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2

indolizino opfuser unknown

c,1,Ring,Ring1,c,2,c,3,n,4,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2

oxindole|oxindol root root

N,1,Ring,Ring1,C,2,(=,x,O,x,),x,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ri
ng1,Ring,Ring2

indoline|indolin root root

N,1,Ring,Ring1,C,2,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2

isat root root

N,1,Ring,Ring1,C,2|alpha,(=O),x,C,3|beta,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,
c,7a,Ring,Ring1,Ring,Ring2

isoindoline|isoindolin root root

C,1,Ring,Ring1,N,2,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2

indane|indan|hydrindene|hydrind root root

C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1,Ring,Ring2

hydrindantin root root O=C(c2c1cccc2)C(C1=O)(O)C(C3=O)(O)C(c4c3cccc4)=O,x

alloxantin root root OC1(C2(C(NC(NC2=O)=O)=O)O)C(NC(NC1=O)=O)=O,x

ninhydrin root root

C,1,(=O),x,Ring,Ring1,C,2,(=O),x,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a
,Ring,Ring1,Ring,Ring2

tetral root root

C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing,Ring1,Ring,Ring2

decal root root

C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,C,4,C,10,Ring,Ring2,C,5,C,6,C,7,C,8,C,9,Ri
ng,Ring1,Ring,Ring2

hexalin root root C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1

quinol|chinol|quinolin|chinolin|leucol root root

n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1,Ring,Ring2

quinolin|chinolin opfuser unknown

n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1,Ring,Ring2

carbostyril|carbostyryl root root

n,1,Ring,Ring1,c,2|b|beta,(O),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
g,Ring1,Ring,Ring2

isocarbostyril|isocarbostyryl root root

c,1,(O),x,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
g,Ring1,Ring,Ring2

lepid root root

n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,(C),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
g,Ring1,Ring,Ring2

cinchonin loveracid root

c,4,Ring,Ring1,c,3,c,2,n,1,c,8a,Ring,Ring2,c,8,c,7,c,6,c,5,c,4a,Ring,Ring1,Ring,
Ring2

quino|chino opfuser unknown
n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1,Ring,Ring2
quinald|chinald root root
C,a|alpha,Ring,Ring3,.,.,x,n,1,Ring,Ring1,c,2|b|beta,Ring,Ring3,c,3,c,4,c,4a,Ring,
Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
xanthur root root
C,a|alpha,Ring,Ring3,.,.,x,n,1,Ring,Ring1,c,2|b|beta,Ring,Ring3,c,3,c,4,(O),x,c,4a
,Ring,Ring2,c,5,c,6,c,7,c,8,(O),x,c,8a,Ring,Ring1,Ring,Ring2
quinoliz|chinoliz root root
c,1,Ring,Ring1,c,2,c,3,c,4,n,5,Ring,Ring2,c,6,c,7,c,8,c,9,c,8a,Ring,Ring2,Ring,R
ing1
quinazol|chinazol root root
n,1,Ring,Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1,Ring,Ring2
quinazol|chinazol|quinazolino opfuser unknown
n,1,Ring,Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1,Ring,Ring2
isoquinol|isochinol root root
c,1|a|alpha,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing,Ring1,Ring,Ring2
isoquino|isochino opfuser unknown
c,1|a|alpha,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing,Ring1,Ring,Ring2
cinnol root root
n,1,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1,Ring,Ring2
quinoxal|chinoxal|phenpiaz root root
n,1,Ring,Ring1,c,2|b|beta,c,3,n,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1,Ring,Ring2
arsinol root root
[as],1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,R
ing1,Ring,Ring2
isoarsinol root root
c,1|a|alpha,Ring,Ring1,[as],2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8
a,Ring,Ring1,Ring,Ring2
phosphinol root root
p,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1,Ring,Ring2
isophosphiol root root
c,1|a|alpha,Ring,Ring1,p,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing,Ring1,Ring,Ring2
pterid root root
n,1,Ring,Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring,Ring2,n,5,c,6,c,7,n,8,c,8a,Ring,Ring
1,Ring,Ring2
phthalazine|phthalazin root root
c,1|a|alpha,Ring,Ring1,n,2|b|beta,n,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing,Ring1,Ring,Ring2
phthalhydrazide root root
C,x,Ring,Ring1,(=O),x,N,x,N,x,C,x,(=O),x,c,2,Ring,Ring2,c,3,c,4,c,5,c,6,c,1,Ring
,Ring1,Ring,Ring2
fluorene|fluoren root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
diphenyleneiodonium root root
[I+],9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring
3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1

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betacarboline root root
c,1,Ring,Ring1,n,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring,Ring3,n,9|prefhydro,c,9a,Ring,Ring2,Ring,Ring1
carbazole|carbazol root root
n,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
carbazolo|carbazol opfuser unknown
n,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
norharman root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,n,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ri
ng,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmane|harman root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmine|banisterine root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmol root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmalol root root
N,9,Ring,Ring1,C,9a,Ring,Ring2,C,1,(C),x,=,x,N,2,C,3,C,4,C,4a,(,x,=,x,Ring,Ring2
,),x,c,4b,Ring,Ring3,c,5,c,6,c,7,(O),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmaline root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,C,3,C,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmalane|harmalan root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,C,3,C,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,(OC),x,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
phenanthrid root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
,10,c,10a,Ring,Ring3,c,10b,Ring,Ring2,Ring,Ring1
arsanthrid root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,
9,c,10,c,10a,Ring,Ring3,c,10b,Ring,Ring2,Ring,Ring1
benzidine|benzidin root root
N,n,c,4,Ring,Ring1,c,3,c,2,c,1,(,x,c,6,c,5,Ring,Ring1,),x,c,1',Ring,Ring2,c,2',c
,3',c,4',(,x,N,n',),x,c,5',c,6',Ring,Ring2
benzidinium root root
[N+],n,c,4,Ring,Ring1,c,3,c,2,c,1,(,x,c,6,c,5,Ring,Ring1,),x,c,1',Ring,Ring2,c,2
',c,3',c,4',(,x,[N+],n',),x,c,5',c,6',Ring,Ring2
benzidino root root
N,4@n,c,4,Ring,Ring1,c,3,c,2,c,1,(,x,c,6,c,5,Ring,Ring1,),x,c,1',Ring,Ring2,c,2'
,c,3',c,4',(,x,N,n',),x,c,5',c,6',Ring,Ring2
pyrid root root
c,2|o|ortho|a|alpha,Ring,Ring1,c,3|m|meta|b|beta,c,4|p|para|g|gamma,c,5,c,6,n,1|
n,Ring,Ring1
pyrido|pyrid opfuser unknown
c,2|o|ortho|a|alpha,Ring,Ring1,c,3|m|meta|b|beta,c,4|p|para|g|gamma,c,5,c,6,n,1|
n,Ring,Ring1
pyridox root root
C,4,c,x,Ring,Ring1,c,x,(,x,C,5,O,x,),x,c,6,n,1,c,2,(C),x,c,3,(O),x,Ring,Ring1
pyridoxamine|pyridoxamin root root
N,x,C,4,c,x,Ring,Ring1,c,x,(,x,C,5,O,x,),x,c,6,n,1,c,2,(C),x,c,3,(O),x,Ring,Ring
1

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pyraz root root
c,2|o|ortho,Ring,Ring1,c,3|m|meta,Ring,Ring2,.,x,n,1|n,Ring,Ring3,Ring,Ring1,.,x
,n,4|p|para|n',Ring,Ring2,c,5,c,6,Ring,Ring3
pyrazino opfuser unknown
c,2|o|ortho,Ring,Ring1,c,3|m|meta,n,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
pyrimid root root
c,2|o|ortho,Ring,Ring1,n,3|m|meta,c,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
pyrimido|pyrimid opfuser unknown
c,2|o|ortho,Ring,Ring1,n,3|m|meta,c,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
pyridaz root root c,3,Ring,Ring1,c,4,c,5,c,6,n,1|n,n,2|n',Ring,Ring1
pyridazo|pyridazino opfuser unknown
c,3,Ring,Ring1,c,4,c,5,c,6,n,1|n,n,2|n',Ring,Ring1
striazine|striazin|symtriazine|symtriazin root root
c,2,Ring,Ring1,n,3,c,4,n,5,c,6,n,1,Ring,Ring1
astriazine|astriazin|asymtriazine|asymtriazin root root
n,2,Ring,Ring1,c,3,n,4,c,5,c,6,n,1,Ring,Ring1
strioxane|strioxan|symtrioxane|symtrioxan root root
C,2,Ring,Ring1,O,3,C,4,O,5,C,6,O,1,Ring,Ring1
astrioxane|astrioxan|asymtrioxane|asymtrioxan root root
O,2,Ring,Ring1,C,3,O,4,C,5,C,6,O,1,Ring,Ring1
strithiane|strithian|symtrithiane|symtrithian root root
C,2,Ring,Ring1,S,3,C,4,S,5,C,6,S,1,Ring,Ring1
astrithiane|astrithian|asymtrithiane|asymtrithian root root
S,2,Ring,Ring1,C,3,S,4,C,5,C,6,S,1,Ring,Ring1
striazino|symtriazino opfuser unknown
c,2,Ring,Ring1,n,3,c,4,n,5,c,6,n,1,Ring,Ring1
astriazino|asymtriazino opfuser unknown
n,2,Ring,Ring1,c,3,n,4,c,5,c,6,n,1,Ring,Ring1
strioxano|symtrioxano opfuser unknown
C,2,Ring,Ring1,O,3,C,4,O,5,C,6,O,1,Ring,Ring1
astrioxano|asymtrioxano opfuser unknown
O,2,Ring,Ring1,C,3,O,4,C,5,C,6,O,1,Ring,Ring1
strithiano|symtrithiano opfuser unknown
C,2,Ring,Ring1,S,3,C,4,S,5,C,6,S,1,Ring,Ring1
astrithiano|asymtrithiano opfuser unknown
S,2,Ring,Ring1,C,3,S,4,C,5,C,6,S,1,Ring,Ring1
borazine|borazin root root N,1,Ring,Ring1,[B],2,N,3,[B],4,N,5,[B],6,Ring,Ring1
phosphazine|borazin root root n,2,Ring,Ring1,p,3,n,4,p,5,n,6,p,1,Ring,Ring1
pyrrole|pyrrol root root n,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
pyrrolo|pyrrol opfuser unknown n,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
pyrrolid root root N,1,Ring,Ring1,C,2|a|alpha,C,3|b|beta,C,4,C,5,Ring,Ring1
pyrrolidino root root N,4@1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
imidazole|imidazol|glyoxaline|glyoxalin root root
c,2,Ring,Ring1,n,3,c,4,=,x,c,5,n,1|prefhydro,Ring,Ring1
imidazolo|imidazol|imidazo|imidaz opfuser unknown
c,2,Ring,Ring1,n,3,c,4,=,x,c,5,n,1,Ring,Ring1
imidazolid root root C,2,Ring,Ring1,N,3,C,4,C,5,N,1,Ring,Ring1
pyrazole|pyrazol root root n,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
pyrazolo|pyrazol opfuser unknown n,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
tetrazolium root root n,1,Ring,Ring1,[n+],2,n,3,n,4,c,5,Ring,Ring1
pyrazabole|pyrazabol root root
c,1,Ring,Ring1,c,2,c,3,n,3a,n,8a,(,x,[B],8,),x,Ring,Ring1,.,x,[B],4,n,4a,Ring,Ri
ng2,c,5,c,6,c,7,n,7a,Ring,Ring2
isooxazole|isooxazol|isoxazole|isoxazol|isoazole|isoazol root root
o,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
isooxazolo|isooxazol|isoxazolo|isoxazol opfuser unknown
o,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
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isooxazolid|isooxazolid|isoxazolid|isoxazolid|isoazolid|isoazolid root root
O,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
urazole|urazol root root N,1,Ring,Ring1,N,2,C,3,(=O),x,N,4,C,5,(=O),x,Ring,Ring1
pyrazolid root root N,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
furan|fur root root o,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,4,c,5,Ring,Ring1
furo opfuser unknown o,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
furfur root root C,a|alpha,c,2,Ring,Ring1,c,3,c,4,c,5,o,1,Ring,Ring1
then root root C,2,c,x,Ring,Ring1,c,3,c,4,c,5,s,1,Ring,Ring1
furazan root root c,3,Ring,Ring1,c,4,n,5,o,1,n,2,Ring,Ring1
isothiazole|isothiazol root root s,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
isothiazolo|isothiazol opfuser unknown s,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
isosulfonazole|isosulfonazol root root
c,4,Ring,Ring1,c,5,s,1,(=,x,O,x,)(=,x,O,x,),x,n,2,c,3,Ring,Ring1
isoselenazole|isoselenazol root root
[se],1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
isoselenazolo|isoselenazol opfuser unknown
[se],1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
benzisosulfonazole|benzisosulfonazol root root
s,1,(=,x,O,x,)(=,x,O,x,),x,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,
7a,Ring,Ring2,Ring,Ring1
benzsulfonazole|benzsulfonazol root root
s,1,(=,x,O,x,)(=,x,O,x,),x,Ring,Ring1,c,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,
7a,Ring,Ring2,Ring,Ring1
sulfonazole|sulfonazol root root
s,1,(=,x,O,x,)(=,x,O,x,),x,Ring,Ring1,c,2,n,3,c,4,c,5,Ring,Ring1
thiophene|thien root root
c,2|a|alpha,Ring,Ring1,c,3|b|beta,c,4,c,5,s,1,Ring,Ring1
thieno|thien opfuser unknown c,2,Ring,Ring1,c,3,c,4,c,5,s,1,Ring,Ring1
selenophene|selenophen root root [se],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
selenopheno|selenophen opfuser unknown
[se],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
tellurophene|tellurophen root root [Te],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
telluropheno|tellurophen opfuser unknown
[Te],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
piperid root root N,1|n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1
piperidino root root N,4@1|n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1
homopiperid root root N,1|n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,Ring,Ring1
nipecot root root C,a|alpha,C,3,Ring,Ring1,C,4,C,5,C,6,N,1|n,C,2,Ring,Ring1
isonipecot root root C,a|alpha,C,4,Ring,Ring1,C,5,C,6,N,1|n,C,2,C,3,Ring,Ring1
purine|purin root root
n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,n,1,c,6,c,5,Ring,Ring1,R
ing,Ring2
adenine|adenin root root
n,1,Ring,Ring1,c,2,n,3,c,4,(,x,c,5,Ring,Ring2,c,6,(,x,N,n|n6,),x,Ring,Ring1,),x,
n,9,c,8,n,7|prefhydro,Ring,Ring2
piperaz root root N,1|n,Ring,Ring1,C,2,C,3,N,4|n',C,5,C,6,Ring,Ring1
piperazino root root N,4@1|n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,Ring,Ring1
homopiperaz root root N,1|n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,C,7,Ring,Ring1
homopiperazino root root N,4@1|n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,C,7,Ring,Ring1
pyrroliz root root
n,4,Ring,Ring1,Ring,Ring2,c,5,c,6,c,7,c,7a,Ring,Ring1,c,1,c,2,c,3,Ring,Ring2
pentalene|pentalen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring1,Ring,Ring2
pentaleno|pentalen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring1,Ring,Ring2
```

heptalene|heptalen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,5a,Ring,Ring2,c,6,c,7,c,8,c,9,c,10,c,10a,Ring,R
ing1,Ring,Ring2
asindacene|asindacen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring,Ring3,c,8b,Ring,Ring2,Ring,Ring1
sindacene|sindacen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,4a,Ring,Ring3,c,5,c,6,c,7,c,7a,Ring
,Ring3,c,8,c,8a,Ring,Ring2,Ring,Ring1
octalene|octalen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,6a,Ring,Ring2,c,7,c,8,c,9,c,10,c,11,c,12,c,
12a,Ring,Ring1,Ring,Ring2
mevalon root root C,1,C,2,C,3,(,x,C,4,C,5,O,x,),(,x,O,x,),x,C,x
lact|lactyl root root C,1,C,2|alpha|a,(,x,O,x,),x,C,3|b|beta
24d root root
O,1@x,C,x,(=,x,O,x,),x,C,a|alpha,O,x,c,1,Ring,Ring1,c,2,(,x,Cl,x,),x,c,3,c,4,(,x
,Cl,x,),x,c,5,c,6,Ring,Ring1
245t root root
O,1@x,C,x,(=,x,O,x,),x,C,a|alpha,O,x,c,1,Ring,Ring1,c,2,(,x,Cl,x,),x,c,3,c,4,(,x
,Cl,x,),x,c,5,(,x,Cl,x,),x,c,6,Ring,Ring1
dnp|24dnp root root c,4@1,Ring,Ring1,c,x,([N+](=O)[O-
]),x,c,3|m|meta,c,x,([N+](=O)[O-]),x,c,5,c,6,Ring,Ring1
morphol root root C,2,Ring,Ring1,C,3,N,4,C,5,C,6,O,1,Ring,Ring1
morpholino root root O,1,Ring,Ring1,C,2,C,3,N,4@4,C,5,C,6,Ring,Ring1
semicarbazide|semicarbazid root root N,1,N,2,C,x,(=,x,O,3,),x,N,4
semicarbazido root root N,4@1,N,2,C,x,(=,x,O,3,),x,N,4
isosemicarbazide|isosemicarbazid root root N,1,N,2,C,x,(,x,O,3,)=,x,N,4
isosemicarbazido root root N,4@1,N,2,C,x,(,x,O,3,)=,x,N,4
semicarbazono root root N,8@1,N,2,C,x,(=,x,O,3,),x,N,4
carbaz root root C,1,N,2,N,3
acetone|aceton root alkane C,1|a|alpha,C,x,(=O),x,C,3|w|omega
acetylacetone root root C,1,C,2,(=,x,O,x,),x,C,3,C,4,(=,x,O,x,),x,C,5
isobutyrone|isobutyron root root CC(C)C(=O)C(C)C,x
isovalerone|isovaleron root root CC(C)CC(=O)CC(C)C,x
enanthone root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,(=O),x,C,8,
C,9,C,10,C,11,C,12,C,13|w|omega
pelargone root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(=O
),x,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
laurone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,x,(=O),x,C,13,C,14,C,15,
C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23|w|omega
myristone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,x,(=O),x,C,15,
C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27|w|omega
palmitone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,x,(=
O),x,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27,C,28,C,29,C,30,C,31|
w|omega
stearone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C
,17,C,x,(=O),x,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27,C,28,C,29,C,30,C,31,
C,32,C,33,C,34,C,35|w|omega
silatrane|silatran root root
[Si],1,Ring,Ring1,Ring,Ring2,O,2,C,3,C,4,N,5,(,x,C,6,C,7,O,8,Ring,Ring1,),x,C,11
,C,10,O,9,Ring,Ring2

glycoluril root root
N,n|1,Ring,Ring1,C,2,(=,x,O,x,),x,N,n'|3,C,3a,Ring,Ring2,N,n''|4,C,5,(=,x,O,x,),
x,N,n'''|6,C,6a,Ring,Ring1,Ring,Ring2
acetylene|acetylen root root C,1,#,x,C,2
diacetylene root root C,1,#,x,C,2,C,3,#,x,C,4
allophan root trivial C,1,(=,x,O,x,),x,N,2,C,3,(=,x,O,x,),x,N,4
biguanide|biguanid root root N,1,C,x,(=,x,N,2,),x,N,3,C,x,(=,x,N,4,),x,N,5
biuret root root N,1,C,2,(=,x,O,x,),x,N,3,C,4,(=,x,O,x,),x,N,5
carbazone|carbazon root root N,1,N,2,C,3,(=,x,O,x,),x,N,4,=,x,N,5
carbazono root root N,4@1,N,2,C,3,(=,x,O,x,),x,N,4,=,x,N,5
carbodiazone|carbodiazon root root N,1,=,x,N,2,C,3,(=,x,O,x,),x,N,4,=,x,N,5
carbodiazono root root N,4@1,=,x,N,2,C,3,(=,x,O,x,),x,N,4,=,x,N,5
carbodiimide|carbodiimid root root N,n|1,=,x,C,x,=,x,N,n'|3
sulfurdiimide|sulfurdiimid root root N,n|1,=,x,S,x,=,x,N,n'|3
carbonohydrazide|carbonohydrazid|carbohydrazide|carbohydrazid|carbazide|carbazid
root root N,1,N,2,C,3,(=,x,O,x,),x,N,4,N,5
carbonohydrazido|carbohydrazido|carbazido root root
N,4@1,N,2,C,x,(=,x,O,x,),x,N,4,N,5
isocarbonohydrazide|isocarbonohydrazid root root
N,1,N,2,C,x,(,x,O,x,)=,x,N,4,N,5
isocarbonohydrazido root root N,4@1,N,2,C,x,(,x,O,x,)=,x,N,4,N,5
formazan root root N,1,N,2,=,x,C,3,N,4,=,x,N,5
guanidine|guanidin root root N,1|n,C,x,(,x,N,3|n',),x,=,x,N,2|n''
guanidino|guanido root root N,4@1,C,x,(=,x,N,2,),x,N,3
hydanto|hydant root root C,1,C,2,N,3,C,4,(=,x,O,x,),x,N,5
hydantoin root root
N,1,Ring,Ring1,C,2,(=,x,O,x,),x,N,3,C,4,(=,x,O,x,),x,C,5,Ring,Ring1
rhodanine|rhodanin root root
S,1,Ring,Ring1,C,2,(=,x,S,x,),x,N,3,C,4,(=,x,O,x,),x,C,5,Ring,Ring1
isourea|pseudourea root root N,1|n,=,x,C,x,(,x,O,2,),x,N,3|n'
1isoureido root root N,4@1|n,=,x,C,x,(,x,O,o,),x,N,3|n'
3isoureido root root N,1|n,=,x,C,x,(,x,O,o,),x,N,4@3|n'
isothiourea root root N,1|n,=,x,C,x,(,x,S,s,),x,N,3|n'
isothiouronium root root N,1|n,=,x,C,x,(,x,[S+],s,),x,N,3|n'
1isothioureido root root N,4@1|n,=,x,C,x,(,x,S,s,),x,N,3|n'
3isothioureido root root N,1|n,=,x,C,x,(,x,S,s,),x,N,4@3|n'
isoselenourea root root N,1|n,=,x,C,x,(,x,[Se],se,),x,N,3|n'
isoselenouronium root root N,1|n,=,x,C,x,(,x,[Se+],se,),x,N,3|n'
1isoselenoureido root root N,4@1|n,=,x,C,x,(,x,[Se],se,),x,N,3|n'
3isoselenoureido root root N,1|n,=,x,C,x,(,x,[Se],se,),x,N,4@3|n'
isotellourea root root N,1|n,=,x,C,x,(,x,[Te],te,),x,N,3|n'
isotellourouronium root root N,1|n,=,x,C,x,(,x,[Te+],te,),x,N,3|n'
1isotelluroureido root root N,4@1|n,=,x,C,x,(,x,[Te],te,),x,N,3|n'
3isotelluroureido root root N,1|n,=,x,C,x,(,x,[Te],te,),x,N,4@3|n'
glycer pseudosugar unknown x,x
glycer root root C,1,C,2,(,x,O,a|alpha,),x,C,3,O,b|beta,
pentaerythritol root root O,x,C,x,C,x,(,x,C,x,O,x,),x,(,x,C,x,O,x,),x,C,x,O,x
pentaerythrityl root root C,4@x,C,x,(,x,C,4@x,),x,(,x,C,4@x,),x,C,4@x
alphapinene root root
C,1,Ring,Ring1,Ring,Ring2,C,2,(,x,C,10,)=,x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
betapinene root root
C,1,Ring,Ring1,Ring,Ring2,C,2,(=,x,C,10,),x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
carve|carv|carvene root root
C,2,Ring,Ring1,C,3,C,4,(,x,C,8,(=,x,C,9,),x,C,10,),x,C,5,c,6,c,1,(,x,C,7,),x,Rin
g,Ring1

dihydrocarve|dihydrocarv|carvomenth root root
C,2,Ring,Ring1,C,3,C,4,(,x,C,8,(=,x,C,9,),x,C,10,),x,C,5,C,6,C,1,(,x,C,7,),x,Rin
g,Ring1
carvacr root root
c,2,Ring,Ring1,c,3,c,4,(,x,C,8,(,x,C,9,),x,C,10,),x,c,5,c,6,c,1,(,x,C,7,),x,Ring
,Ring1
betaapinene root root
C,1,Ring,Ring1,Ring,Ring2,C,2,(=,x,C,10,),x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
pinacol root root
O,x,C,x,(,x,C,x,),x,(,x,C,x,),x,C,x,(,x,O,x,),x,(,x,C,x,),x,C,x
pinacolyl root root C,4@x,(,x,C,x,),x,C,x,(,x,C,x,),x,(,x,C,x,),x,C,x
pinacolone root root C,1,C,2,(=,x,O,x,),x,C,3,(,x,C,x,),x,(,x,C,x,),x,C,x
benzopinacole|benzopinacol root root
C,x,(,x,C,x,(,x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,(,x,c,1',Ring,
Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2,),x,(O),x,),x,(,x,c,1'',Ring,Ring3,c,2
'',c,3'',c,4'',c,5'',c,6'',Ring,Ring3,),x,(,x,c,1''',Ring,Ring4,c,2''',c,3''',c,
4''',c,5''',c,6''',Ring,Ring4,),x,O,x
benzopinacolone root root
O=C(C4=CC=CC=C4)C(C2=CC=CC=C2)(C3=CC=CC=C3)C1=CC=CC=C1,x
resorcinol root root
O,o,c,1,Ring,Ring1,c,2,c,3,(,x,O,o',),x,c,4,c,5,c,6,Ring,Ring1
orsellin root root
c,2|o|ortho,Ring,Ring1,c,3,(,x,O,o',),x,c,4|p|para,c,5,(,x,O,o'',),x,c,6,c,1,(C)
,x,Ring,Ring1
olivetol root root
O,x,c,1,Ring,Ring1,c,2,c,3,(,x,O,x,),x,c,4,c,5,(CCCCC),x,c,6,Ring,Ring1
hydroquinone|hydroquinon root root
c,1,Ring,Ring1,Ring,Ring2,c,2,c,3,c,4,Ring,Ring3,c,5,c,6,Ring,Ring1,.,x,O,o,Ring
,Ring2,.,x,O,o',Ring,Ring3
syring root root
C,x,c,1,Ring,Ring1,c,2,c,3,(,x,OC,x,),x,c,4,(,x,O,x,),x,c,5,(,x,OC,x,),x,c,6,Rin
g,Ring1
syringol root root
O,x,c,1,Ring,Ring1,c,2,(OC),x,c,3,c,4,c,5,c,6,(OC),x,Ring,Ring1
pyrogallol root root
O,x,c,1,Ring,Ring1,c,2,(,x,O,x,),x,c,3,(,x,O,x,),x,c,4,c,5,c,6,Ring,Ring1
orcinol root root
O,x,c,1,Ring,Ring1,c,2,c,3,(,x,O,x,),x,c,4,c,5,(,x,C,x,),x,c,6,Ring,Ring1
pyrogallitol root root
O,x,C,1,Ring,Ring1,C,2,(,x,O,x,),x,C,3,(,x,O,x,),x,C,4,C,5,C,6,Ring,Ring1
phloroglucin root root
c,1,Ring,Ring1,c,2,c,3,(,x,O,x,),x,c,4,c,5,(,x,O,x,),x,c,6,Ring,Ring1
phloroglucide root root Oc1cc(O)c(c2cc(O)cc(O)c2)c(O)c1,x
thym root root
c,3,Ring,Ring1,c,2,c,1,(,x,C,x,),x,c,6,c,5,c,4,(,x,C,x,(,x,C,x,),x,C,x,),x,Ring,
Ring1
isopuleg root root
C,x,Ring,Ring1,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,(,x,C,x,(=,x,C,x,),x,C,x,),x,Ring
,Ring1
pyrocatechol|orthocatechol root root
O,x,c,1,Ring,Ring1,c,2,(,x,O,x,),x,c,3,c,4,c,5,c,6,Ring,Ring1
nitrone|nitron root root C,a|alpha,=,x,[N+],n,[O-],x
glyoxime|glyoxim root root C,x,(,x,C,x,=,x,N,x,O,x,),x,=,x,N,x,O,x
coumarine|coumarin|cumarin root root
o,1,Ring,Ring1,c,2,(=,x,O,x,),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
g,Ring1,Ring,Ring2

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isocoumarin|isocumarin root root
C,1,Ring,Ring1,(=,x,O,x,),x,o,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
g,Ring1,Ring,Ring2
coumaran root root
O,1,Ring,Ring1,C,2,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
coumarone|coumaron root root
o,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
2
ayapin root root
o,1,Ring,Ring1,c,2,(=,x,O,x,),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,(,x,COC,x,Ring,R
ing3,),x,c,7,Ring,Ring3,c,8,c,8a,Ring,Ring1,Ring,Ring2
benzhydr root root
C,a|alpha,(,x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,
c,2',c,3',c,4',c,5',c,6',Ring,Ring2
benzoguanamine|benzoguanamin root root
c,1,(,x,Ring,Ring1,n,2,c,3,(,x,N,x,),x,n,4,c,5,(,x,N,x,),x,n,6,Ring,Ring1,),x,c,
1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
trit root root
C,a|alpha,Ring,Ring1,Ring,Ring2,Ring,Ring3,.,x,c,4,Ring,Ring4,Ring,Ring5,.,x,c,4
',Ring,Ring6,Ring,Ring7,.,x,c,4'',Ring,Ring8,Ring,Ring9,.,x,c,3,Ring,Ring4,c,2,c
,1,Ring,Ring1,c,6,c,5,Ring,Ring5,.,x,c,3',Ring,Ring6,c,2',c,1',Ring,Ring2,c,6',c
,5',Ring,Ring7,.,x,c,3'',Ring,Ring8,c,2'',c,1'',Ring,Ring3,c,6'',c,5'',Ring,Ring
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ureth root root N,n,C,x,(=,x,O,x,),x,O,x,C,x,C,x
chalcone|chalcon root root
C,a|alpha,(,x,C,x,(=,x,O,x,),x,c,1',Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Rin
g1,),x,=,x,C,b|beta,c,1,Ring,Ring2,c,2,c,3,c,4,c,5,c,6,Ring,Ring2
deoxybenzoin root root
C,a|alpha,(,x,C,x,(=O),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',
Ring,Ring2,=,x,C,2',c,3',c,4',c,5',c,6',Ring,Ring2
thiurammonosulfide|thiurammonosulfid root root
N,n,C,x,(=,x,S,x,),x,S,x,C,x,(=,x,S,x,),x,N,n'
thiuramdisulfide|thiuramdisulfid root root
N,n,C,x,(=,x,S,x,),x,SS,x,C,x,(=,x,S,x,),x,N,n'
thiuramtrisulfide|thiuramtrisulfid root root
N,n,C,x,(=,x,S,x,),x,SSS,x,C,x,(=,x,S,x,),x,N,n'
thiuramtetrasulfide|thiuramtetrasulfid root root
N,n,C,x,(=,x,S,x,),x,SSSS,x,C,x,(=,x,S,x,),x,N,n'
mercuran root root S=C(SSC(N(C)C)=S)N(C)C,x
diacetamide|diacetamid root root
N,n,(,x,C,x,(,x,=,x,O,x,),x,C,x,),x,C,x,(,x,=,x,O,x,),x,C,x
triacetamide|triacetamid root root
N,x,(,x,C,x,(,x,=,x,O,x,),x,C,x,),x,(,x,C,x,(,x,=,x,O,x,),x,C,x,),x,C,x,(,x,=,x,
O,x,),x,C,x
dibenzamide|dibenzamid root root
N,n,(,x,C,x,(,x,=,x,O,x,),x,c,x,Ring,Ring1,ccccc,x,Ring,Ring1,),x,C,x,(,x,=,x,O,
x,),x,c,x,Ring,Ring2,ccccc,x,Ring,Ring2
tribenzamide|tribenzamid root root
N,x,(,x,C,x,(,x,=,x,O,x,),x,c,x,Ring,Ring1,ccccc,x,Ring,Ring1,),x,(,x,C,x,(,x,=,
x,O,x,),x,c,x,Ring,Ring2,ccccc,x,Ring,Ring2,),x,C,x,(,x,=,x,O,x,),x,c,x,Ring,Rin
g3,=,x,ccccc,x,Ring,Ring3
fulvene|fulven root root
C,6,=,x,C,5,Ring,Ring1,C,1,=,x,C,2,C,3,=,x,C,4,Ring,Ring1
stilbene|stilben root root
C,b|beta|a'|alpha',(=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|pa

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ra,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,c,2'|o'|ortho',c,3'|m'|meta',c,4'|p'|p
ara',c,5',c,6',Ring,Ring2
stilbestrol|stilboestrol root root
C,b|beta,(=,x,C,a|alpha,c,1,Ring,Ring1,c,2,c,3,c,4,(O),x,c,5,c,6,Ring,Ring1,),x,
c,1',Ring,Ring2,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring2
hexestrol root root
C,b|beta,(CC)(,x,C,a|alpha,(CC),x,c,1,Ring,Ring1,c,2,c,3,c,4,(O),x,c,5,c,6,Ring,
Ring1,),x,c,1',Ring,Ring2,c,2',c,3',c,4',(O),x,c,5',c,6',Ring,Ring2
benzil root root
C(=O),x,(,x,C(=O),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',Ring,
Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
antipyr|antipyrene|phenazone root root
C,4,Ring,Ring1,C,5,(=O),x,N,1,(,x,N,2,(,x,C,x,),x,C,3,(,x,C,x,),x,=,x,Ring,Ring1
,),x,c,1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
glycid root root C,1,C,2|b|beta,Ring,Ring1,C,3,O,x,Ring,Ring1
ketene|keten root root C=C=O,1
diketene|diketen root root C=C1CC(=O)O1,x
adamant root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,Ring,Ring3,C,4,C,5,(,x,C,6,C,7,(,x,C,8,Ring,Ri
ng1,),x,C,10,Ring,Ring3,),x,C,9,Ring,Ring2
noradamant root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,Ring,Ring3,C,4,C,5,(,x,C,6,C,7,(,x,C,8,Ring,Ri
ng1,),x,Ring,Ring3,),x,C,9,Ring,Ring2
hexamethylenetetramine|hexamethylenetetramin root root
N,1,Ring,Ring1,Ring,Ring2,C,2,N,3,Ring,Ring3,C,4,N,5,(,x,C,6,N,7,(,x,C,8,Ring,Ri
ng1,),x,C,10,Ring,Ring3,),x,C,9,Ring,Ring2
pentamethylenetetramine|pentamethylenetetramin root root N12CNCN(CNC1)C2,x
fulvalene|fulvalen root root
c,2,Ring,Ring1,(,x,c,3,c,4,c,5,c,1,Ring,Ring1,)=,x,c,2',Ring,Ring2,c,3',c,4',=,x
,c,5',c,1',Ring,Ring2
tetrathiafulvalene|tetrathiafulvalen root root
C,2,Ring,Ring1,(,x,S,3,C,4,=,x,C,5,S,1,Ring,Ring1,)=,x,C,2',Ring,Ring2,S,3',C,4'
,=,x,C,5',S,1',Ring,Ring2
tetraselenafulvalene|tetrathiafulvalen root root
C,2,Ring,Ring1,(,x,[Se],3,C,4,=,x,C,5,[Se],1,Ring,Ring1,)=,x,C,2',Ring,Ring2,[Se
],3',C,4',=,x,C,5',[Se],1',Ring,Ring2
labd root natural
C,1,Ring,Ring1,C,2,C,3,[C@@],4,(,x,C,18,),x,(,x,C,19,),x,[C@@],5,([H]),x,Ring,Ri
ng2,C,6,C,7,[C@],8|a-r,(,x,C,17,),x,[C@@],9|a-
b,(,x,[C@],10,Ring,Ring2,Ring,Ring1,C,20,),x,C,11|a-
t,C,12,[C@],13,(,x,C,16,),x,C,14,C,15
ambros root natural C,2,Ring,Ring1,C,3,C,4,[C@@],5|a-
b,Ring,Ring2,(,x,C,15,),x,C,6|a-
r,[C@],7,(,x,C,11,(,x,C,12,),x,C,13,),x,C,8,C,9,[C@],10,(,x,C,14,),x,[C@@],1|a-
t,([H]),x,Ring,Ring2,Ring,Ring1
cedr root natural [C@@],2,Ring,Ring1,(,x,C,12,),x,C,3,C,4,[C@],5|a-
b,([H]),x,Ring,Ring2,[C@@],6|a-
r,(,x,C,13,),x,(,x,C,14,),x,[C@],7,(,x,C,11,Ring,Ring3,),x,[C@],8,(,x,C,15,),x,C
,9,C,10,[C@@],1|a-t,Ring,Ring1,Ring,Ring2,Ring,Ring3
cedrol root natural OC1(C)C3CC2(C(C3(C)C)CCC2C)CC1,x
apotrichothec root natural
O,1,Ring,Ring1,[C@],12,Ring,Ring2,(,x,C,13,),x,C,2,C,3,C,4,[C@@],5|a-
r,(,x,C,14,),x,Ring,Ring2,[C@],6|a-
b,(,x,C,15,),x,Ring,Ring3,C,7,C,8,C,9,(,x,C,16,),x,C,10,[C@],11|a-
t,([H]),x,Ring,Ring3,Ring,Ring1

germacr root natural
C,1,Ring,Ring1,C,2,C,3,[C@],4,(,x,C,15,),x,C,5,C,6,[C@],7,(,x,C,11,(,x,C,12,),x,
C,13,),x,C,8,C,9,[C@@],10,(,x,C,14,),x,Ring,Ring1
podocarpa|podocarp root steroid
C,1,Ring,Ring1,C,2,C,3,[C@@],4,(,x,C,15|18,),x,(,x,C,16|19,),x,C,5,Ring,Ring2,C,
6,C,7,C,8,Ring,Ring3,C,14,C,13,C,12,C,11,C,9,Ring,Ring3,[C@@],10,(,x,C,17,),x,Ri
ng,Ring1,Ring,Ring2
palustr root natural
C,x,Ring,Ring4,.,,x,CC(C)C(CC3)=CC2=C3[C@]1(C)C(CC2)[C@@],x,Ring,Ring4,(C)CCC1,x
gedun root natural
C,1,Ring,Ring1,C,2,C,3,C,4,(,x,C,30,),x,(,x,C,31,),x,C,5,Ring,Ring2,C,6,C,7,C,8,
Ring,Ring3,(,x,C,x,),x,C,14,Ring,Ring4,C,15,C,16,O,x,C,17,(,x,C,20,Ring,Ring5,C,
x,O,x,C,23,C,22,Ring,Ring5,),x,C,13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,R
ing3,C,10,(,x,C,19,),x,Ring,Ring2,Ring,Ring1
eudesm root natural
C,1,Ring,Ring1,C,2,C,3,[C@],4,(C),x,[C@@],5,([H]),x,Ring,Ring2,C,6,[C@],7|a-
r,(,x,C,11,(C),x,C,x,),x,C,8|a-b,C,9|a-t,[C@],10,(C),x,Ring,Ring2,Ring,Ring1
trichotheca|trichothec root natural C,3,Ring,Ring1,C,4,[C@@],5|a-
r,(,x,C,14,),x,Ring,Ring2,[C@],6|a-
b,(,x,C,15,),x,Ring,Ring3,C,7,C,8,[C@],9,(,x,C,10,[C@],11|a-
t,([H]),x,Ring,Ring3,O,1,[C@],2,Ring,Ring1,[C@],12,Ring,Ring2,C,13,),x,C,16
scirpenol root natural [C@],3,(O),x,Ring,Ring1,C,4,[C@@],5|a-
r,(,x,C,14,),x,Ring,Ring2,[C@],6|a-
b,(,x,C,15,),x,Ring,Ring3,C,7,C,8,C,9,(=,x,C,10,[C@],11,([H]),x,Ring,Ring3,O,1,[
C@],2,Ring,Ring1,[C@@],12,Ring,Ring2,(,x,O,x,Ring,Ring4,),x,C,13,Ring,Ring4,),x,
C,16
prosta|prost root natural C,1,C,2,C,3,C,4,C,5,C,6,C,7,[C@@H],8|a-
t,(,x,C,9,C,10,C,11,Ring,Ring1,),x,[C@H],12|a-b,Ring,Ring1,C,13|a-
r,C,14,C,15,C,16,C,17,C,18,C,19,C,20
phorbol root natural O,x,[C@@],13,1(,x,[C@@H],12,2O)[C@H]([C@@](C=C,a-
t,Ring,Ring3,CO)([H])[C@@](O)([C@@](C=C(C)C4=O)([H]),x,[C@],4|a-b,4(O)C,a-
r,3)[C@@H]2C)[C@@]1(C)C,x
tigli|tiglia root natural
C,13,Ring,Ring1,(,x,C,12,Ring,Ring2,),x,[C@H],x,(,x,[C@@],8,(,x,C,7,=,x,C,6|a-
t,Ring,Ring3,C,20,),x,([H]),x,C,9,(,x,[C@@],10,(,x,C,1,C,2,(C),x,C,3,Ring,Ring4,
),x,([H]),x,C,4|a-b,Ring,Ring4,C,5|a-
r,Ring,Ring3,),x,[C@@H],x,Ring,Ring2,C,x,),x,[C@@],x,Ring,Ring1,(C),x,C,x
glutathionereduced root root
O=C(NCC(,x,O,1@x,)=O)C(C,x,S,s,)NC(CCC(N)C(,x,O,1@x,)=O)=O,x
glutathione root root
O=C(NCC(O)=O)[C@H](CSSC[C@H](NC(CC[C@H](N)C(O)=O)=O)C(NCC(O)=O)=O)NC(CC[C@H](N)C
(O)=O)=O,x
sphingosin|sphingosine|dihydrosphingosin|dihydrosphingosine pseudosugar unknown
x,x
sphingosin|sphingosine root root
O,x,C,1,C,2,(,x,N,n,),x,C,3,(O),x,C,4,=,x,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,1
3,C,14,C,15,C,16,C,17,C,18
dihydrosphingosin|dihydrosphingosine root root
O,x,C,1,C,2,(,x,N,x,),x,C,3,(O),x,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,
14,C,15,C,16,C,17,C,18
phenacetin root root CCOC1=CC=C(NC(C)=O)C=C1,x
xanthotoxin root root COC1=C(OC3=O)C(C=C3)=CC2=C1OC=C2,x
troxonium root root O=C(C1=CC(OC)=C(C(OC)=C1)OC)OCC[N+](CC)(CC)CC,x
triclopyr root root O,1@x,C(=O)COC(N=C(Cl)C(Cl)=C1)=C1Cl,x
thonzonium|tonzonium root root
COC1=CC=C(C=C1)CN(C2=NC=CC=N2)CC[N+](C)(C)CCCCCCCCCCCCCCCC,x
tolonium root root NC1=CC2=C(N=C(C=C3)C(S2)=CC3=[N+](C)C)C=C1C,x

tolazoline root root C(c1ccccc1)C2=NCCN2,x
tiodonium root root ClC(C=C2)=CC=C2[I+]C1=CC=CS1,x
tiemonium root root C[N+]1(CCC(C2=CC=CC=C2)(C3=CC=CS3)O)CCOCC1,x
tiametonium root root CC[N+](C)(CCSCC[N+](C)(CC)C)C,x
tibezonium root root
CC[N+](CC)(C)CCSC2=NC1=C(N=C(C4=CC=C(C=C4)SC3=CC=CC=C3)C2)C=CC=C1,x
tetramisole root root C1CSC2=NC(c3ccccc3)CN12,x
suxethonium root root CC[N+](C)(CCOC(CCC(OCC[N+](C)(CC)C)=O)=O)C,x
suxamethonium|succinylcholine root root
C[N+](C)(CCOC(CCC(OCC[N+](C)(C)C)=O)=O)C,x
sultroponium root root C[N+]1(C2CCC1CC(OC(C(C3=CC=CC=C3)CO)=O)C2)CCCS([O-
])(=O)=O,x
stilonium root root CC[N+](CC)(CCOC2=CC=C(C=C2)C=CC1=CC=CC=C1)CC,x
spiropentane root root
C,1,Ring,Ring1,C,2,C,3,Ring,Ring1,Ring,Ring2,C,4,C,5,Ring,Ring2
sorbitane|sorbitan root root O[C@@H]([C@@H]1[C@H](O)[C@@H](O)CO1)CO,x
sesamol root root OC1=CC(OCO2)=C2C=C1,x
sepazonium root root
ClC1=CC(Cl)=C(COC(C4=CC=C(C=C4Cl)Cl)CN2C=C[N+](CCC3=CC=CC=C3)=C2)C=C1,x
scopoletin root root o1c(=O)ccc2cc(OC)c(O)cc12,x
salbutamol root root CC(C)(NCC(C1=CC(CO)=C(O)C=C1)O)C,x
saccharin|glucarin|saccharine|glucarine root root C(=O)1NS(=O)(=O)c2ccccc21,x
saccharide|saccharinate root root C(=O)1[N-]S(=O)(=O)c2ccccc21,x
imazethapyr|pursuit root root
O=C1NC(C2=C(C(,x,O,1@x,)=O)C=C(CC)C=N2)=NC1(C)C(C)C,x
pyridoxine|pyridoxin root root CC1=NC=C(CO)C(CO)=C1O,x
prolonium|hydroxytriethoium root root C[N+](C)(C)CC(O)C[N+](C)(C)C,x
prodeconium root root CCCOC(C[N+](C)(CCOCCCCCCCCCCOCC[N+](C)(CC(OCCC)=O)C)C)=O,x
procaine root root Nc1ccc(C(OCCN(CC)CC)=O)cc1,x
procainamide|procaineamide root root Nc1ccc(C(NCCN(CC)CC)=O)cc1,x
pirdonium root root CC1=CC=C(C(C3=CC=CC=C3)OCC2CCCC[N+]2(C)C)C=C1,x
pentolonium|pentolinium root root C[N+]1(CCCCC[N+]2(C)CCCC2)CCCC1,x
lytensium|penthonium|pentamethonium root root C[N+](C)(C)CCCCC[N+](C)(C)C,x
penoctonium root root O=C(OCC[N+](CC)(CC)CCCCCCCC)C(C2CCCC2)C1CCCC1,x
acetaminophen|paracetamol root root O=C(NC(C=C1)=CC=C1O)C,x
amiben|chloramben root root O,1@x,C(=O)C1=C(Cl)C(N)=CC(Cl)=C1,x
chlorfenac root root O,1@x,C(=O)CC(C(Cl)=CC=C1Cl)=C1Cl,x
actinonin root root OCC1N(C(C(C(C)C)NC(C(CC(NO)=O)CCCCC)=O)=O)CCC1,x
aminopropylon root root O=C1N(c2ccccc2)N(C)C(C)=C1NC(C(C)N(C)C)=O,x
azamethonium root root CC[N+](C)(C)CCN(C)CC[N+](C)(C)CC,x
benzathonium|benzethonium root root
CC(C)(C1=CC=C(OCCOCC[N+](C)(C)CC2=CC=CC=C2)C=C1)CC(C)(C)C,x
methylbenzathonium|methylbenzethonium root root
CC(C)(C1=CC(C)=C(OCCOCC[N+](C)(C)CC2=CC=CC=C2)C=C1)CC(C)(C)C,x
benzilonium root root O=C(OC1C[N+](CC)(CC1)CC)C(C2=CC=CC=C2)(C3=CC=CC=C3)O,x
bevonium root root OC(C(OCC3[N+](C)(C)CCCC3)=O)(C2=CC=CC=C2)C1=CC=CC=C1,x
carpronium root root COC(CCC[N+](C)(C)C)=O,x
carvone root root CC(C1=O)=CCC(C1)C(C)=C,x
cetrimonium root root CCCCCCCCCCCCCCCC[N+](C)(C)C,x
chloraminophen root root ClCCN(C1=CC=C(CCCC(O)=O)C=C1)CCCl,x
chloraminophenamide root root O=S(N)(C1=C(Cl)C=C(N)C(S(=O)(N)=O)=C1)=O,x
chloramphenicol root root OC[C@@H](NC(C(Cl)Cl)=O)[C@@H](C1=CC=C([N+]([O-
])=O)C=C1)O,x
chlorphonium root root CCCC[P+](CCCC)(CCCC)CC1=CC=CC=C1,x
ciclonium root root CC[N+](CC)(CCOC(C1CC2CC1C=C2)(C3=CC=CC=C3)C)C,x
cyclopyrronium root root CC[N+]1(CCC(OC(C(C3=CC=CC=C3)C2CCCC2)=O)C1)C,x
cypion root root CCCC1CCCC1,x

decamethonium root root C[N+](C)(C)CCCCCCCCCC[N+](C)(C)C,x
deditonium root root
CC(C1=CC=C(C=C1OCC[N+](C)(CCCCCCCCCC[N+](C)(CCOC2=CC(C)=CC=C2C(C)C)C)C)C)C,x
denatonium root root CC[N+](CC(NC(C(C)=CC=C2)=C2C)=O)(CC)CC1=CC=CC=C1,x
dicyclopentadiene root root
C,1,Ring,Ring1,c,2,c,3,C,3a,Ring,Ring2,C,4,Ring,Ring3,c,5,c,6,C,7,(,x,C,x,Ring,Ring3,),x,C,7a,Ring,Ring2,Ring,Ring1
dimecolonium root root CC1CCCC([N+]1(C)C)C(OCC[N+](C)(C)C)=O,x
dimidium root root c1cc(N)cc2c(c3ccccc3)[n+](C)c4cc(N)ccc4c21,x
dinoseb root root CC(C(C=C([N+]([O-])=O)C=C1[N+]([O-])=O)=C1O)CC,x
disilethylene root root [Si],1,C,2,C,3,[Si],4
disiquonium root root C[N+](CCCCCCCCCC)(CCC[Si](OC)(OC)OC)CCCCCCCCCC,x
dotefonium root root CN(C(C(C2=CC=CC=C2)(C3=CC=CS3)O)=O)CC[N+]1(CCCC1)C,x
ebdc root root S,1@x,C(NCCNC(,x,S,1@x,)=S)=S,x
edrophonium root root CC[N+](C)(C1=CC=CC(O)=C1)C,x
emepronium root root CC[N+](C)(C(CC(C2=CC=CC=C2)C1=CC=CC=C1)C)C,x
fentonium root root
C[N+]3(C4CCC3CC(OC(C(C5=CC=CC=C5)CO)=O)C4)CC(C1=CC=C(C2=CC=CC=C2)C=C1)=O,x
fludazonium root root
O=C(C1=CC=C(F)C=C1)CN(C=C2)C=[N+]2CC(C4=C(C=C(C=C4)Cl)Cl)OCC3=C(C=C(C=C3)Cl)Cl,x
furacrin loveracid root CC1=CC(C=C2C(C(CC)=C)=O)=C(C=C2C)O1,x
fosamine|fosamin root root O=P(O)(OCC)C(N)=O,x
fubrogonium root root CC[N+](CC)(CCC(OC(C1=CC=C(O1)Br)=O)C)C,x
furtrethonium root root C[N+](C)(C)CC1=CC=CO1,x
glufosinate|glufosinat root root CP(O)(CCC(C(,x,O,1@x,)=O)N)=O,x
glycopyrronium root root OC(C1CCCC1)(C2=CC=CC=C2)C(OC(CC3)C[N+]3(C)C)=O,x
glyphosate|glyphosat root root O,1@x,C(CNCP(O)(O)=O)=O,x
heteronium root root C[N+]1(CCC(OC(C(C2=CC=CC=C2)(C3=CC=CS3)O)=O)C1)C,x
hexafluoronium root root
C[N+](C)(C2C1=C(C3=C2C=CC=C3)C=CC=C1)CCCCC[N+](C)(C6C4=C(C5=CC=CC=C56)C=CC=C4)C,x
hexamethonium root root C[N+](C)(CCCCCC[N+](C)(C)C)C,x
hexasonium root root C[S+](CCOC(C(C2=CC=CC=C2)C1CCCC1)=O)C,x
hexopyrronium root root C[N+]1(CCC(OC(C(C2CCCC2)(C3=CC=CC=C3)O)=O)C1)C,x
imazaquin root root CC(C1(N=C(C3=NC2=CC=CC=C2C=C3C(,x,O,1@x,)=O)NC1=O)C)C,x
isoluminol root root NC1=CC=C2C(C(NNC2=O)=O)=C1,x
mebezonium root root C[N+](C)(C1CCC(CC2CCC([N+](C)(C)C)CC2)CC1)C,x
mecetronium root root CCCCCCCCCCCCCCCCCC[N+](C)(CC)C,x
chloramben root root O,1@x,C(=O)C1=C(N)C(Cl)=CC(Cl)=C1,x
nitronium root root O=[N+]=O,x
nifuroxime root root ON=Cc1ccc(o1)[N+](=O)[O-],x
octafonium root root CC[N+](CCOC1=CC=C(C=C1)CC(C)(CC(C)C)C)(CC2=CC=CC=C2)CC,x
otilonium root root
CCCCCCCCOC1=CC=CC=C1C(NC2=CC=C(C(OCC[N+](CC)(CC)C)=O)C=C2)=O,x
oxitefonium root root CC[N+](CC)(CCOC(C(C1=CC=CC=C1)(C2=CC=CS2)O)=O)C,x
pxydipentonium root root C[NH+](CCCCCOCCCCC[N+](C)(C)C)C,x
oxyphenonium root root CC[N+](CC)(CCOC(C(C1CCCCC1)(C2=CC=CC=C2)O)=O)C,x
oxypyrronium root root C[N+]1(CCCC1COC(C(C2CCCCC2)(C3=CC=CC=C3)O)=O)C,x
oxysonium root root C[S+](CCOC(C(C1CCCCC1)(C2=CC=CC=C2)O)=O)C,x
amezinium root root COC1=CC(N)=CN=[N+]1C2=CC=CC=C2,x
amenzpyrinium root root CN(C(OC1=CC=C[N+](CC2=CC=CC=C2)=C1)=O)C,x
carcainium root root C[N+](CC(NC1=CC=CC=C1)=O)(CC(NC2=CC=CC=C2)=O)C,x
clonidine root root
c,p,Ring,Ring1,c,m,c,x,(Cl),x,c,x,(NC2=NCCN2),x,c,x,(Cl),x,c,x,Ring,Ring1
dequalinium root root
CC1=CC(N)=C2C(C=CC=C2)=[N+]1CCCCCCCCCC[N+](C(C)=C3)=C(C=CC=C4)C4=C3N,x
elliptinium root root CC(C2=C1C=C[N+](C)=C2)=C(C3=C4C=CC(O)=C3)C(N4)=C1C,x

fazadinium root root
CC5=C(N(C6=[N+]5C=CC=C6)N=NN3C(C2=CC=CC=C2)=C([N+]4=C3C=CC=C4)C)C1=CC=CC=C1,x
fenpiverinium root root C[N+]1(CCC(C2=CC=CC=C2)(C3=CC=CC=C3)C(N)=O)CCCCC1,x
methanthelinium root root O=C(C2C3=C(C=CC=C3)OC1=CC=CC=C12)OCC[N+](CC)(C)CC,x
methylthioninium root root CN(C1=CC([S+]=C(C=C(N(C)C)C=C3)C3=N2)=C2C=C1)C,x
metocinium root root C[N+](C)(CCOC(C(C1=CC=CC=C1)(C2=CC=CC=C2)O)=O)C,x
nicotine root root CN1C(C2=CC=CN=C2)CCC1,x
nolinium root root ClC(C=C3)=C(Cl)C=C3NC2=CC1=CC=CC=[N+]1C=C2,x
pentolinium root root C[N+]1(CCCCC[N+]2(C)CCCC2)CCCC1,x
prifinium root root CC[N+]2(CCC(C2C)=C(C3=CC=CC=C3)C1=CC=CC=C1)CC,x
promethazine root root CC(N(C)C)CN1C3=C(C=CC=C3)SC2=C1C=CC=C2,x
pyrvinium root root
CN(C1=CC4=C([N+](C)=C(C=C4)C=CC2=C(C)N(C3=CC=CC=C3)C(C)=C2)C=C1)C,x
rosaniline|rosanilin root root
N=C(C=C3)C=CC3=C(C2=CC=C(N)C(C)=C2)C1=CC=C(N)C=C1,x
senfol root root N=C=S,x
tartrazine root root O=C1N(C3=CC=C([S](=O)([O-])=O)C=C3)N=C(C([O-
])=O)C1N=NC2=CC=C([S](=O)([O-])=O)C=C2.[Na+].[Na+].[Na+],x
thonzylaminium root root COc2cc(cc2)CN(c1ncccn1)CC[N+](C)C,x
trantelinium root root C[N+]1(C2CCC1CC(OC(C4C3=CC=CC=C3OC5=C4C=CC=C5)=O)C2)C,x
trimethidinium root root CC1(C2CCC1(C[N+](CCC[N+](C)(C)C)(C2)C)C)C,x
thenium root root C[N+](CCOC2=CC=CC=C2)(C)CC1=CC=CS1,x
menrium|tropium|librium|solium root root [O-
][N+](CC(NC)=N3)=C(C2=C3C=CC(Cl)=C2)C1=CC=CC=C1,x
oxapropanium root root C[N+](C)(C)CC1OCOC1,x
furium root root [O-][N+](C1=CC=C(C2=CSC(NC(C)=O)=N2)O1)=O,x
tropylium root root C1=CC=C[C+]C=C1,x
acetaminophen root root Oc1ccc(cc1)NC(=O)C,x
acetur root root CCNC(=O)C,x
afurolol root root CC(C)(NCC(COC(C=CC=C1CO2)=C1C2=O)O)C,x
agallol root root COCC[Hg]Cl,x
alizarin root root O=C(c2ccccc23)c1c(O)c(O)ccc1C3=O,x
allantoin root root O=C(N1)NC(NC(N)=O)C1=O,x
amantanium root root CCCCCCCCCC[N+](C)(CCOC(C23CC1CC(C3)CC(C2)C1)=O)C,x
aminopentamide root root CC(N(C)C)CC(C1=CC=CC=C1)(C2=CC=CC=C2)C(N)=O,x
amprolium root root CCCC2=NC=C(C(N)=N2)C[N+]1=C(C)C=CC=C1,x
aporph root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,C,4,C,5,N,6,(C),x,C,6a,Ring,Ring3,C,7,c,7
a,Ring,Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,11b,Ring,Ring1,c,11c,Ring,Ring
2,Ring,Ring3
noraporph root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,C,4,C,5,N,6,C,6a,Ring,Ring3,C,7,c,7a,Ring
,Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,11b,Ring,Ring1,c,11c,Ring,Ring2,Ring
,Ring3
aspirin root root O=C(O)c1ccccc1OC(C)=O,x
azaspirium root root
COC(C1=C(C(OC)=C23)C=CO1)=C3OC5=C(C[N+]4(CC5=C)CCCCC4)C2=O,x
bephenium root root C[N+](CCOC1=CC=CC=C1)(CC2=CC=CC=C2)C,x
berb root root c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,C,5,C,6,N,7|a-
r,Ring,Ring3,C,8,c,8a,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,C,13|a-
t,C,13a|a-b,Ring,Ring3,c,13b,Ring,Ring2,Ring,Ring1
bidimazium root root
CN(C1=CC=C(C=CC2=[N+](C)C(C3=CC=C(C4=CC=CC=C4)C=C3)=CS2)C=C1)C,x
bretylium root root CC[N+](C)(CC1=C(Br)C=CC=C1)C,x
busulfan root root O=S(OCCCCOS(=O)(C)=O)(C)=O,x
carazolol root root OC(CNC(C)C)COC1=CC=CC2=C1C(C=CC=C3)=C3N2,x
clofilium root root CCCCCCC[N+](CC)(CCCCC1=CC=C(C=C1)Cl)CC,x

datelliptium root root
CC1=C4C(C=C[N+](CC[NH+](CC)CC)=C4)=C(C)C3=C1C2=C(N3)C=CC(O)=C2,x
demecarium root root
CN(C(OC2=CC=CC([N+](C)(C)C)=C2)=O)CCCCCCCCCCN(C(OC1=CC=CC([N+](C)(C)C)=C1)=O)C,x
dibromantin root root CC(C(N1Br)=O)(N(Br)C1=O)C,x
digermin root root O=[N+]([O-])C1=CC(C(F)(F)F)=CC([N+]([O-])=O)=C1N(CCC)CCC,x
diphenhydramine root root CN(C)CCOC(C2=CC=CC=C2)C1=CC=CC=C1,x
dithizone root root S=C(NNC2=CC=CC=C2)N=NC1=CC=CC=C1,x
dopamine root root
NCC,x,c,1,Ring,Ring1,c,2,c,3,(O),x,c,4,(O),x,c,5,c,6,Ring,Ring1
etipirium root root C[N+]1(CCOC(C(C2=CC=CC=C2)(C3=CC=CC=C3)O)=O)CCCC1,x
fench root root
C,2|a|alpha,Ring,Ring1,C,3,(C)(C),x,C,4,(,x,C,5,C,6,C,1,Ring,Ring2,(C),x,Ring,Ring1,),x,C,7,Ring,Ring2
feniodium root root ClC2=CC=C(C(Cl)=C2)[I+]C1=CC=C(C=C1Cl)Cl,x
flutropium root root C[N+]1(C2CCC1CC(OC(C(C3=CC=CC=C3)(C4=CC=CC=C4)O)=O)C2)CCF,x
furazolium root root [O-][N+](C1=CC=C(C2=CSC3=[N+]2CCN3)O1)=O,x
halopenium root root CC(C1=CC(Cl)=C(C=C1OCCC[N+](C)(CC2=CC=C(C=C2)Br)C)C)C,x
hexafluorenium root root
C[N+](C)(C2C1=C(C3=C2C=CC=C3)C=CC=C1)CCCCC[N+](C)(C6C4=C(C5=CC=CC=C56)C=CC=C4)C,x
hexocyclium root root C[N+]1(CCN(CC(C2CCCCC2)(C3=CC=CC=C3)O)CC1)C,x
ethidium|homidium root root
NC(C=C3)=CC2=C3C1=CC=C(N)C=C1C(C4=CC=CC=C4)=[N+]2CC,x
indenolol root root CC(NCC(COC2=C1C=CCC1=CC=C2)O)C,x
ionone|ionon|alphaionon|alphaionone root root O=C(C)C=CC1c(C)cCCC1(C)C,x
betaionone|betaionon root root O=C(C)C=CC1=C(C)CCCC1(C)C,x
isometamidium root root
CC[N+]4=C(C2=C(C5=CC=C(C=C45)N)C=CC(NN=NC3=CC=CC(C(N)=N)=C3)=C2)C1=CC=CC=C1,x
isophor root root C,1,Ring,Ring1,C,2,C,3,(C),x,C,4,C,5,(C)(C),x,C,6,Ring,Ring1
isophorone root root
O=,x,C,1,Ring,Ring1,C,2,=,x,C,3,(C),x,C,4,C,5,(C)(C),x,C,6,Ring,Ring1
lapirium root root O=C(NCCOC(CCCCCCCCCC)=O)C[N+]1=CC=CC=C1,x
methylbenactyzium root root OC(C1=CC=CC=C1)(C2=CC=CC=C2)C(OCC[N+](CC)(C)CC)=O,x
benactyzine root root CCN(CCOC(C(C1=CC=CC=C1)(C2=CC=CC=C2)O)=O)CC,x
miripirium root root CCCCCCCCCCCCC[N+]1=CC=C(C)C=C1,x
neopentylglycol root root OCC(C)(C)CO,x
nioxime root root ON=C(CCCC1)C1=NO,x
oxapium root root C[N+]1(CC2COC(C3CCCCC3)(C4=CC=CC=C4)O2)CCCCC1,x
oxolin root root CC2=CN(CC)C1=CC(OCO3)=C3C=C1C2=O,x
oxprenolol root root CC(NCC(COC1=CC=CC=C1OCC=C)O)C,x
oxybenzone root root O=C(C1=CC=CC=C1)C(C=CC(OC)=C2)=C2O,x
penbutolol root root OC(CNC(C)(C)C)COC1=C(C2CCCC2)C=CC=C1,x
pentacynium root root
C[N+](CCCCC(C1=CC=CC=C1)(C2=CC=CC=C2)C#N)(CC[N+]3(CCOCC3)C)C,x
pentazocine root root CC2C3(C)C1=CC(O)=CC=C1CC2N(CC=C(C)C)CC3,x
phenacetur root root CCNC(=O)Cc1ccccc1,x
phencyclidine|angeldust root root c1(C2(N3CCCCC3)CCCCC2)ccccc1,x
pinaverium root root COC4=CC(Br)=C(C=C4OC)C[N+]3(CCOCC3)CCOCCC1CCC2CC1C2(C)C,x
piperylene root root C=CC=CC,x
piproctanylium root root CC(C)CCCC(C)CC[N+]1(CC=C)CCCCC1,x
piprocurarium root root CC[N+](CC)(CCOCCOC(C([N+]2(CCCCC2)C)C1=CC=CC=C1)=O)C,x
pranolium root root CC(C)[N+](C)(C)CC(O)COC1=C2C(C=CC=C2)=CC=C1,x
pretamazium root root
CC[N+]3=C(SC=C3C4=CC=C(C5=CC=CC=C5)C=C4)C=CC1=CC=C(N2CCCC2)C=C1,x
propanolol root root OC(CNC(C)C)COC1=C2C(C=CC=C2)=CC=C1,x

propidium root root
C[N+](CC)(CC)CCC[N+](C3=C2C=CC(N)=C3)=C(C4=CC=CC=C4)C1=C2C=CC(N)=C1,x
prospidium root root ClCC(O)CN3CC[N+]2(CC3)CC[N+]1(CC2)CCN(CC1)CC(O)CCl,x
pyritidium root root
CC1=CC(NC2=CC(C(C3=CC=C(C=C3)N)=[N+](C5=CC(N)=CC=C45)C)=C4C=C2)=NC(N)=[N+]1C,x
quinomethionate|chinomethionate root root O=C3SC2=NC1=CC(C)=CC=C1N=C2S3,x
salicin root root O[C@H]1O[C@@H](OC2=CC=CC=C2CO)[C@H](O)[C@@H](O)[C@@H]1O,x
serenium root root CCOC(C=C2)=CC=C2N=NC1=CC=C(N)C=C1N,x
sintropium root root CCCC(C(OC1CC2CCC([N+]2(C(C)C)C)C1)=O)CCC,x
stilbazium root root
CC[N+]1=C(C=CC5=CC=C(C=C5)N4CCCC4)C=CC=C1C=CC3=CC=C(C=C3)N2CCCC2,x
timepidium root root COC2CC(C[N+](C)(C2)C)=C(C3=CC=CS3)C1=CC=CS1,x
tipetropium root root CCC[N+]1(C2CCC1CC(OC4C3=CC=CC=C3CSC5=CC=CC=C45)C2)C,x
tiquizium root root C[N+]13CCCCC1CCC(C3)=C(C4=CC=CS4)C2=CC=CS2,x
trimethylsilyldifluoride root root [Si-](C)(C)(C)(F)F,x
tricine root root OCC(CO)(CO)NCC(O)=O,x
toliodium root root CC2=CC=C(C=C2)[I+]C1=CC=C(C=C1)C,x
trazium root root OC1(C4=CC=C(C=C4)Cl)NC=N[N+]3=C1C2=CC=CC=C2C=C3,x
trepirium root root C[N+](C)(CCOC(C1CCC[N+]1(C)C)=O)C,x
tropolone|tropalone root root
O=,x,c,1,Ring,Ring1,c,7,c,6,c,5,c,4,c,3,c,2,Ring,Ring1,O,x
tyloxapol root root NCCc1ccc(O)cc1,x
urocan root root
C,x,C,a|alpha,=,x,C,b|beta,c,4,Ring,Ring1,n,3,c,2,n,1|prefhydro,c,5,Ring,Ring1
verbenone root root O=C1C(C2)C(C)(C)C2C(C)=C1,x
yohimb|yohimbin loveracid root C,x,Ring,Ring6,.,x,N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,C,5,C,6,C,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,C,21,[C@@],20,([H]),x,Ring,Ring5,C,19,C,18,[C@H],17,
(O),x,[C@H],16,Ring,Ring6,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
yohimb|yohimba root root N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,C,5,C,6,C,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,C,21,[C@@],20,([H]),x,Ring,Ring5,C,19,C,18,C,17,C,16
,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
yohimbine|yohimbin root root N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,C,5,C,6,C,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,C,21,[C@@],20,([H]),x,Ring,Ring5,C,19,C,18,[C@H],17,
(O),x,[C@H],16,(C(=O)OC),x,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
oxayohimb|oxayohimba root root N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,C,5,C,6,C,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,C,21,[C@@],20,([H]),x,Ring,Ring5,C,19,C,18,O,17,C,16
,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
morphinan root natural c,1,Ring,Ring1,c,2,c,3,c,4,c,12|a-t,Ring,Ring2,[C@],13|a-
b,Ring,Ring4,Ring,Ring3,C,5,C,6,C,7,C,8,[C@@],14,Ring,Ring3,([H]),x,[C@],9|a-
r,(,x,N,17,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
morphine root natural
c,1,Ring,Ring1,c,2,c,3,(O),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
t,Ring,Ring2,[C@],13|a-
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,[C@@],6,(O),x,C,7,=,x,C,8,[C@@],14,Ring,R
ing3,([H]),x,[C@],9|a-
r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
codeine root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
t,Ring,Ring2,[C@],13|a-

b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,[C@@],6,(O),x,C,7,=,x,C,8,[C@@],14,Ring,R
ing3,([H]),x,[C@],9|a-
r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
codeinone root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
t,Ring,Ring2,[C@],13|a-b
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(=O),x,C,7,=,x,C,8,[C@@],14,Ring,Ring
3,([H]),x,[C@],9|a-
r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
dihydrocodeinone|hydrocodeinone root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
t,Ring,Ring2,[C@],13|a-b
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(=O),x,C,7,=,x,C,8,[C@@],14,Ring,Ring
3,([H]),x,[C@],9|a-
r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
thebacon root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,O,x,Ring,Ring5,),x,c,12|a-
t,Ring,Ring2,[C@],13|a-b
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(OC(=O)C),x,=,x,C,7,C,8,[C@@],14,Ring
,Ring3,([H]),x,[C@],9|a-
r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
ergoline|ergolin root natural
n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H]),x,Ring,Ring3,N,6,C,7,C,8|a-
t,C,9|a-b,C,10|a-
r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring
,Ring4
lyserg root natural
C,x,Ring,Ring5,.,.,x,n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H]),x,Ring,Rin
g3,N,6,(C),x,C,7,[C@],8|a-t,Ring,Ring5,C,9|a-b,=,x,C,10|a-
r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring
,Ring4
lysergide root natural
C,x,Ring,Ring5,(=O)N(CC)CC.,x,n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H])
,x,Ring,Ring3,N,6,(C),x,C,7,[C@],8|a-t,Ring,Ring5,C,9|a-b,=,x,C,10|a-
r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring
,Ring4
ergotaman root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,N,x,[
C@],2',Ring,Ring5,C,3',N,4',Ring,Ring6,C,5',C,6',N,7',Ring,Ring7,C,8',C,9',C,10'
,[C@],11',([H]),x,Ring,Ring7,[C@@H],12',Ring,Ring6,O,1',Ring,Ring5
ergocornine|ergocornin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C)
,x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@]
,12',(O),x,Ring,Ring6,O,1',Ring,Ring5
ergocorninine|ergocorninin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O)
,x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C
),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@
],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
ergocristine|ergocristin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(Cc9ccc

cc9),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[
C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
ergocryptine|ergocryptin|ergocriptine|ergocriptin|alphaergocryptine|alphaergocry
ptin|alphaergocriptine|alphaergocriptin root natural c,a-t,Ring,Ring1,c,a-
b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C
),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@
],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|
bergocryptin|bergocriptine|bergocriptin root natural c,a-t,Ring,Ring1,c,a-
b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)CC
),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@
],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
ergocryptinine|ergocryptinin|ergocriptinine|ergocriptinin|alphaergocryptinine|al
phaergocryptinin|alphaergocriptinine|alphaergocriptinin root natural c,a-
t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O)
,x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)
C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@
@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
betaergocryptinine|betaergocryptinin|betaergocriptinine|betaergocriptinin|bergoc
ryptinine|bergocryptinin|bergocriptinine|bergocriptinin root natural c,a-
t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O)
,x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C
C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@
@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
ergosine|ergosin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,
C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12
',(O),x,Ring,Ring6,O,1',Ring,Ring5
ergotamine|ergotamin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(Cc9ccccc9)
,x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@]
,12',(O),x,Ring,Ring6,O,1',Ring,Ring5
bromocryptine|bromocryptin|bromocriptine|bromocriptin root natural c,a-
t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
l,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,(Br),x,Ring,Ring4,),x,c,x,Ring,Ring3,c,
x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,1
8,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',
(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Rin
g7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
ecgonidine|ecgonidin root root
[C@@],x,([H]),x,Ring,Ring1,Ring,Ring2,C,x,c,x,c,x,(,x,C,x,(=O),x,O,1@x,),x,[C@],
x,([H]),x,(,x,N,x,(C),x,Ring,Ring1,),x,C,x,C,x,Ring,Ring2

ecgonine|ecgonin root root
[C@@],x,([H]),x,Ring,Ring1,Ring,Ring2,C,x,[C@H],x,(O),x,[C@H],x,(,x,C,x,(=O),x,O
,1@x,),x,[C@],x,([H]),x,(,x,N,x,(C),x,Ring,Ring1,),x,C,x,C,x,Ring,Ring2
methylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(C),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,c
,2',c,3',[n+],4',(C),x,c,5',c,6',Ring,Ring2
ethylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(CC),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,
c,2',c,3',[n+],4',(CC),x,c,5',c,6',Ring,Ring2
benzylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(Cc3ccccc3),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring
,Ring2,c,2',c,3',[n+],4',(Cc4ccccc4),x,c,5',c,6',Ring,Ring2
pheneturide root root O=C(N)NC(C(CC)C1=CC=CC=C1)=O,x
lactide|dilactide root root CC(OC1=O)C(OC1C)=O,x
gallion root root OC(C(Cl)=CC([N+]([O-
])=O)=C3)=C3N=NC1=C(S(=O)(O)=O)C=C(C=C(S(=O)(O)=O)C=C2N)C2=C1O,x
clofibr root root CC(C)(OC1=CC=C(C=C1)Cl)C,x
paraben root root O,1@x,C(C1=CC=C(O)C=C1)=O,x
edetate|versenate|edta root root
O,1@x,C(CN(CC(,x,O,1@x,)=O)CCN(CC(,x,O,1@x,)=O)CC(,x,O,1@x,)=O)=O,x
fusar root root CC1=CC=C(CCCC)C=N1,x
lironion root root COC1=CC=C(OC2=CC=C(C=C2)NC(N(C)C)=O)C=C1,x
thionalide root root O=C(CS)NC2=CC1=CC=CC=C1C=C2,x
tolperisone root root CC(C(C2=CC=C(C)C=C2)=O)CN1CCCCC1,x
valethamate root root CCC(C(C(OCC[N+](CC)(CC)C)=O)C1=CC=CC=C1)C,x
secbutabarbital|butalan root root O=C(N1)NC(C(C(C)CC)(CC)C1=O)=O,x
furalan root root O=C(N2)N(CC2=O)N=CC1=CC=C([N+]([O-])=O)O1,x
boc|tboc root nprotect C,4@x,(=O)OC(C)(C)C,x
z-nprot root nprotect C,4@x,(=O)OCc1ccccc1,x
msoc root nprotect C,4@x,(=O)OCCS(=O)(=O)C,x
cbz root nprotect
C,4@x,(=O)OC,x,C,1,Ring,Ring1,=,x,C,2,C,3,=,x,C,4,C,5,=,x,C,6,Ring,Ring1
fmoc root nprotect C,4@x,(=O)OCC1C2=CC=CC=C(C3=CC=CC=C13)2,x
dansyl root nprotect S,4@x,(C2=CC=CC1=C(N(C)C)C=CC=C12)(=O)=O,x
dabsyl root nprotect S,4@x,(c1ccc(N=Nc2ccc(N(C)C)cc2)cc1)(=O)=O,x
bansyl root nprotect S,4@x,(C2=CC=CC1=C(N(CCCC)CCCC)C=CC=C12)(=O)=O,x
nps root nprotect S,4@x,c1c([N+](=O)[O-])cccc1,x
tfa root nprotect C,4@x,(=O)C(F)(F)F,x
acm root nprotect C,4@x,NC(=O)C,x
phacm root nprotect C,4@x,NC(=O)Cc1ccccc1,x
creatine root root CN(C(N)=N)CC(O)=O,x
panthenol root root CC(CO)(C(C(NCCCO)=O)O)C,x
alanate root root [AlH4-],x
cyanamide root root NC#N,x
eprolin root root CC1=C2C(OC(CCCC(C)CCCC(C)CCCC(C)C)(C)CC2)=C(C)C(C)=C1O,x
eserine|physostigmine root root O=C(NC)OC1=CC=C(N(C)C3C2(C)CCN3C)C2=C1,x
prolan root root CC([N+]([O-])=O)C(C2=CC=C(Cl)C=C2)C1=CC=C(Cl)C=C1,x
tropanserin root root CN1C2CCC1CC(OC(C3=CC(C)=CC(C)=C3)=O)C2,x
butanserin root root FC1=CC=C(C(C4CCN(CC4)CCCCN3C(NC2=CC=CC=C2C3=O)=O)=O)C=C1,x
amiprol|domalium|kiatrium|levium|relanium|tensium|umbrium|velium|valium root
root O=C1CN=C(C3=CC=CC=C3)C2=C(C=CC(Cl)=C2)N1C,x
prolate root root S=P(OC)(OC)SCN1C(C(C=CC=C2)=C2C1=O)=O,x
adaprolol root root CC(NCC(COC4=CC=C(C=C4)CC(OCCC23CC1CC(C3)CC(C2)C1)=O)O)C,x
agmatine root root NC(NCCCCN)=N,x
algolysin root root CCC(C(C1=CC=CC=C1)(C2=CC=CC=C2)CC(C)N(C)C)=O.[H]Cl,x
altanserin root root FC1=CC=C(C(C2CCN(CCN4C(NC3=CC=CC=C3C4=O)=S)CC2)=O)C=C1,x

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angelicin root root
c,1,Ring,Ring1,c,2,o,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,(=O),
x,o,9,c,9a,Ring,Ring3,c,9b,Ring,Ring2,Ring,Ring1
asparagusate root root OC(C1CSSC1)=O,x
aspartame root root O=C(OC)C(NC(C(N)CC(O)=O)=O)CC1=CC=CC=C1,x
bisoprolol root root OC(CNC(C)C)COC1=CC=C(COCCOC(C)C)C=C1,x
bornaprolol root root OC(CN(CC)C)CC1=CC=CC=C1C2C3CCC(C3)C2,x
broncholysin root root OC(C(CS)NC(C)=O)=O,x
bunaprolast root root CCCCC2=C(OC(C)=O)C1=CC=CC=C1C(OC)=C2,x
butethal root root CCCCC(C(NC1=O)=O)(C(N1)=O)CC,x
capsaicin root root O=C(CCCC/C=C/C(C)C)NCc1ccc(O)c(OC)c1,x
carbachol root root C[N+](C)(C)CCOC(N)=O,x
carlsoprol root root CC(COC(N)=O)(CCC)COC(NC(C)C)=O,x
caryolysine root root ClCCN(C)CCCl,x
chloral root root O=CC(Cl)(Cl)Cl,x
chloralhydrate root root OC(O)C(Cl)(Cl)Cl,x
bromal root root O=CC(Br)(Br)Br,x
bromalhydrate root root OC(O)C(Br)(Br)Br,x
chrysanthemum|chrysanthem root root C1C(C=C(C)C)C(C)(C)1,x
celiprolol root root OC(CNC(C)(C)C)COC1=C(C(C)=O)C=C(NC(N(CC)CC)=O)C=C1,x
cinanserin root root CN(CCCSC1=CC=CC=C1NC(C=CC2=CC=CC=C2)=O)C,x
clemeprol root root CN(CC(C(C2=CC=CC(Cl)=C2)C1=CC=CC=C1)O)C,x
coumal root root Cc1ccc(=O)oc1,x
creatinine root root N1C(=N)N(C)CC(=O)1,x
cyclen root root
N,1,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,N,7,C,8,C,9,N,10,C,11,C,12,Ring,Ring1
cyprolidol root root OC(C3=CC=CC=C3)(C4=CC=CC=C4)C1CC1C2=CC=NC=C2,x
deprol root root CC(COC(N)=O)(CCC)COC(N)=O,x
dibuprol root root CCCCOCC(O)COCCCC,x
eburnamonine root root O=C2N(c3ccccc34)C1=C4CCN5C1C(CCC5)(CC)C2,x
exaprolol root root CC(NCC(COC1=CC=CC=C1C2CCCCC2)O)C,x
epichlorohydrin root root ClCC1CO1,x
epithiochlorohydrin root root ClCC1CS1,x
epifluorohydrin root root FCC1CO1,x
epibromohydrin root root BrCC1CO1,x
erban root root O=C(CC)NC1=CC(Cl)=C(Cl)C=C1,x
ethacryn root root CCOC1=C(Cl)C(Cl)=C(C=C1)C(C(CC)=C)=O,x
farmiserina|cycloserine|cycloserin|micoserina root root NC(CON1)C1=O,x
fascaplysin root root O=C(C5=C4C=CC=C5)C1=[N+]4C=CC2=C1NC3=C2C=CC=C3,x
febuprol root root CCCCOCC(O)COC1=CC=CC=C1,x
fermine root root O=C(OC)C1=CC=CC=C1C(OC)=O,x
fertilysin root root O=C(C(Cl)Cl)NCCCCCCCNC(C(Cl)Cl)=O,x
formamidinedisulfide root root NC(SSC(N)=N)=N,x
ftorafur root root O=C(N1)N(C2CCCO2)C=C(F)C1=O,x
geneserine|eseridine root root CC23C1=CC(OC(NC)=O)=CC=C1N(C)C20N(CC3)C,x
glutim|pidol root root C,x,C,5,Ring,Ring1,C,4,C,3,C,2,(=O),x,N,1,Ring,Ring1
hexethal root root O=C(N1)NC(C(CCCCCC)(CC)C1=O)=O,x
ibuprofen root root C(C)(C)Cc1ccc(cc1)C(C)C(=O)O,x
indameth root root ClC(C=C3)=CC=C3C(N2C(C)=C(CC(O)=O)C1=CC(OC)=CC=C12)=O,x
iomeprol root root CN(C1=C(I)C(C(NCC(CO)O)=O)=C(I)C(C(NCC(CO)O)=O)=C1I)C(CO)=O,x
iridocin root root NC(C1=CC(CC)=NC=C1)=S,x
isatoicanhydride root root
O=C(O2)c,1,Ring,Ring1,c,6,c,5,c,4,c,3,c,2,Ring,Ring1,NC2=O,x
isoprene root root C=CC(=C)C,x
isoxaprolol root root CC1=NOC(C=CC2=CC=CC=C2OCC(CNC(C)(C)C)O)=C1,x
ketanserin root root FC1=CC=C(C(C2CCN(CCN4C(NC3=CC=CC=C3C4=O)=O)CC2)=O)C=C1,x

limonene root root
C,7,c,1,Ring,Ring1,c,2,C,3,C,4,(,x,C,8,(=,x,C,9,),x,C,10,),x,C,5,C,6,Ring,Ring1
meprol|meproleaf root root CC(COC(N)=O)(CCC)COC(N)=O,x
metoprolol root root COCCCC1=CC=C(OCC(O)CNC(C)C)C=C1,x
mianserin root root CN1CCN3C(C2=C(CC4=CC=CC=C34)C=CC=C2)C1,x
moprolol root root COC(C=CC=C1)=C1OCC(CNC(C)C)O,x
myrtan root root CC1CCC(C2)C(C)(C)C21,x
myrten root root CC1=CCC(C2)C(C)(C)C21,x
nicainoprol root root CC(NCC(COC1=CC=CC2=C1N(C(C3=CC=CN=C3)=O)CCC2)O)C,x
nitrogendioxide root root O,x,=,x,[N+],16@x,[O-],x
nitricoxide root root N,32@x,=O,x
nitrousoxide root root N#[N+][O-],x
ozone|trioxygen root root O=[O+][O-],x
oxaceprol root root CC(N1CC(CC1C(O)=O)O)=O,x
pelanserin root root O=C2NC1=CC=CC=C1C(N2CCCN3CCN(C4=CC=CC=C4)CC3)=O,x
phencyclone root root O=c(c(c5c3c4ccccc4c6ccccc56)c2ccccc2)c3c1ccccc1,x
phenindione root root O=C(C2=C1C=CC=C2)C(C3=CC=CC=C3)C1=O,x
propranolol root root OC(CNC(C)C)COc1cccc2ccccc12,x
psoralen root root
o,1,Ring,Ring1,c,2,(=O),x,c,3,c,4,c,x,Ring,Ring2,c,5,c,x,Ring,Ring3,c,4',c,5',o,
x,c,x,Ring,Ring3,c,8|8',c,x,Ring,Ring2,Ring,Ring1
thioct root root CCCCCC1SSCC1,x
phosphoramide|phosphorustriamide root root P(=O),x,(,x,N,n,)(,x,N,n',),x,N,n''
pyrophosphoramide|diphosphoramide root root
P(=O),x,(,x,N,n,)(,x,N,n',),x,O,x,P(=O),x,(,x,N,n'',),x,N,n'''
prolintane root root CCCC(N2CCCC2)CC1=CC=CC=C1,x
resorufin root root
c,7,Ring,Ring1,c,6,c,5a,Ring,Ring2,o,5,c,4a,Ring,Ring3,c,4,c,3,(=O),x,c,2,c,1,c,
10a,Ring,Ring3,n,10,c,9a,Ring,Ring2,c,9,c,8,Ring,Ring1
retin root root
C,15,C,14,=,x,C,13,(,x,C,20,),x,C,12,=,x,C,11,C,10,=,x,C,9,(,x,C,19,),x,C,8,=,x,
C,7,C,6,Ring,Ring1,=,x,C,5,(,x,C,18,),x,C,4,C,3,C,2,C,1,(,x,C,16,)(,x,C,17,),x,R
ing,Ring1
ritanserin root root
CC(N=C1SC=CN12)=C(CCN3CCC(CC3)=C(C5=CC=C(C=C5)F)C4=CC=C(C=C4)F)C2=O,x
seganserin root root
CC(NC1=CC=CC=[N]12)=C(CCN3CCC(CC3)=C(C5=CC=C(C=C5)F)C4=CC=C(C=C4)F)C2=O,x
vinylsulfurol root root C=CC1=C(C)N=CS1,x
teoprolol root root
CC(NCC(COC3=CC=CC4=C3C=C(C)N4)O)CCN1C=NC(N(C(N2C)=O)C)=C1C2=O,x
terbuprol root root COCC(COC(C)(C)C)O,x
thyropropion aminoacid ine
C,x,C,a|alpha,C,b|beta,C,1,Ring,Ring2,=,x,C,2|ortho,C,3|m|meta,=,x,C,4,(,x,O,x,C
,1',Ring,Ring3,=,x,C,2',C,3',=,x,C,4',(,x,O,x,),x,C,5',=,x,C,6',Ring,Ring3,),x,C
,5,=,x,C,6,Ring,Ring2
thyroacet aminoacid ine
C,x,C,a|alpha,C,1,Ring,Ring2,=,x,C,2|ortho,C,3|m|meta,=,x,C,4,(,x,O,x,C,1',Ring,
Ring3,=,x,C,2',C,3',=,x,C,4',(,x,O,x,),x,C,5',=,x,C,6',Ring,Ring3,),x,C,5,=,x,C,
6,Ring,Ring2
toliprolol root root CC(NCC(COC1=CC=CC(C)=C1)O)C,x
tolysin root root O=C(C1=C3C(C=CC(C)=C3)=NC(C2=CC=CC=C2)=C1)OCC,x
tomoxiprole root root COC1=CC=C(C4=NC2=C(N4C(C)C)C=CC3=CC=CC=C23)C=C1,x
tricyclene|tricyclen root root CC12C(C2C3)CC3C1(C)C,x
triprolidine root root CC1=CC=C(C(C3=NC=CC=C3)=CCN2CCCC2)C=C1,x
tranexam root root C[C@H]1CC[C@H](CN)CC1,x
tropicamide root root OCC(C(N(CC)CC2=CC=NC=C2)=O)C1=CC=CC=C1,x
zipeprol root root COC(C3=CC=CC=C3)CN1CCN(CC(C(C2=CC=CC=C2)OC)O)CC1,x

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thioindigo root root O=C1C4=C(C=CC=C4)SC1=C2SC(C=CC=C3)=C3C2=O,x
theophyllol root root O=C1C2=C(NC=N2)N(C)C(N1C)=O.O=C([O-])C.[Na+],x
synephrine root root OC1=CC=C(C(O)CNC)C=C1,x
sulfathiazole root root NC1=CC=C(S(NC2=NC=CS2)(=O)=O)C=C1,x
sulfadiazine root root
O=S(N,x,c,2,Ring,Ring1,n,3,c,4,c,5,c,6,n,1,Ring,Ring1,)(C2=CC=C(N)C=C2)=O,x
strychnine root root O=C(C5)N(C4C2(CC7)C(N7C6)CC3C6=CCOC5C34)C1=C2C=CC=C1,x
squalane root root CC(CCCCC(C)CCCC(C)CCCC(C)C)CCCC(C)CCCC(C)C,x
squalene root root CC(C)=CCC\C(C)=C\CC\C(C)=C\CC\C=C(C)\CC/C=C(CCC=C(C)C)/C,x
spermine|neuridine|musculamine|gerontine root root NCCCNCCCCNCCCN,x
spermidine root root NCCCNCCCCN,x
scopolamine root root CN1C2CC(OC(C(CO)c4ccccc4)=O)CC1C3C2O3,x
genoscopolamine root root C[N+]([O-])1C2CC(OC(C(CO)C4=CC=CC=C4)=O)CC1C3C2O3,x
sendachromeal root root O=C(C(C(O)=O)=C2)C=CC2=C(C)C1=CC(C(O)=O)=C(O)C=C1,x
sorb root root C,1,C,2,=,x,C,3,C,4,=,x,C,5,C,6
quercitin root root OC1=CC(C(O3)=C(O)C(C2=C3C=C(O)C=C2O)=O)=CC=C1O,x
pulegone root root CC1CC(=O)C(=C(C)C)CC1,x
benzindopyrine|benzindopyrin root root c(CCc2ccncc2)(cn3Cc4ccccc4)c1c3cccc1,x
benziodarone|benziodaron root root O=C(c3cc(I)c(O)c(I)c3)c2c1ccccc1oc2CC,x
benzopyrronium root root C[N+]1(CCC(OC(C(c2ccccc2)(c3ccccc3)O)=O)C1)C,x
benzothiozane|benzothiozan root root O=C(C)Nc1ccc(C=NNC(N)=S)cc1,x
benzpiperylone|benzpiperylon root root
O=C1C(Cc3ccccc3)=C(c4ccccc4)NN1C2CCN(C)CC2,x
benzpyrinium root root CN(C(Oc1c[n+](Cc2ccccc2)ccc1)=O)C,x
benzquinamide|benzquinamid root root
CCN(C(C3CN2CCc1c(C2CC3OC(C)=O)cc(OC)c(OC)c1)=O)CC,x
benzthiazide|benzthiazid root root
O=S2(c1cc(S(N)(=O)=O)c(Cl)cc1N=C(CSCc3ccccc3)N2)=O,x
benzthiazuron root root O=C(NC)Nc2sc1ccccc1n2,x
methabenzthiazuron root root O=C(NC)N(C)c2sc1ccccc1n2,x
benzvalene|benzvalen root root C13C=CC2C1C23,x
abscis|absciss root root
C,1,C,2,=,x,C,3,(C),x,C,4,=,x,C,5,C,6,(C(C)(C1)C)(C(C)=CC1=O)O,x
mobenzoxamine|mobenzoxamin root root
COc1ccc(C(c4ccccc4)OCCN3CCN(CC3)CCCC(c2ccc(F)cc2)=O)cc1,x
quinuclidine|quinuclidin root root
N,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,C,8,Ring,Ri
ng2
uranine root root O=C3C=CC2=C(C4=CC=CC=C4C([O-])=O)C1=CC=C([O-
])C=C1CC2=C3.[Na+].[Na+],x
thorin root root OC1=C(N=NC3=C([As](O)(O)=O)C=CC=C3)C2=C(C=C(S([O-
])(=O)=O)C=C2)C=C1S([O-])(=O)=O.[Na+].[Na+],x
furaneol root root CC1OC(C)=C(O)C1=O,x
bicine|bicin root root O=C(O)CN(CCO)CCO,x
indanthrone root root
O=C(C3=C2C=CC=C3)C1=C(NC4=CC=C(C6=O)C(C(C7=CC=CC=C67)=O)=C4N5)C5=CC=C1C2=O,x
methone|dimedone root root
C,1,(=O),x,Ring,Ring1,C,2,C,3,(=O),x,C,4,C,5,(C)(C),x,C,6,Ring,Ring1
acrinol root root NC1=C(C=C(OCC)C=C3)C3=NC2=C1C=CC(N)=C2.CC(O)C(O)=O,x
danthron root root O=C(C2=C1C=CC=C2O)C(C(O)=CC=C3)=C3C1=O,x
caffeine|caffein root root O=C(N(C)C2=C1N(C)C=N2)N(C)C1=O,x
betahistine root root CNCCc1ncccc1,x
pyranine root root [O-]S(C(C=C4O)=C1C=CC2=C(S([O-])(=O)=O)C=C(S([O-
])(=O)=O)C3=CC=C4C1=C23)(=O)=O.[Na+].[Na+].[Na+],x
abiet root root C,x,[C@],a-
r,2(C)C1[C@]([C@@](CCc(C(C)C)c3)([H])C3=CC1)(C,x,C,a-t,C,a-b,2)C,x

betulin loveracid root
C[C@@]45CC[C@@]3(C)[C@]2(C)CC[C@@]1([H])C(C)(C)[C@@H](O)CC[C@]1(C)[C@@]2([H])CCC
3[C@@]4([H])[C@H](C(C)=C)CC5,x
betulin root root
OC[C@@]45CC[C@@]3(C)[C@]2(C)CC[C@@]1([H])C(C)(C)[C@@H](O)CC[C@]1(C)[C@@]2([H])CC
C3[C@@]4([H])[C@H](C(C)=C)CC5,x
caluros root root CC(C)(c1ccccc1)CC=C(C)C,x
thymine|thymin|uracil|orot|isoorot|cytosine|isocytosine|guanine|xanthine|hypoxan
thine pseudosugar unknown x,x
thymine|thymin root root
N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,(=O),x,c,5,(C),x,c,6,Ring,Ring1
uracil root root N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,(=O),x,c,5,c,6,Ring,Ring1
orot root root C,x,c,6,Ring,Ring1,N,1,C,2,(=O),x,N,3,C,4,(=O),x,c,5,Ring,Ring1
isoorot root root
C,x,c,5,Ring,Ring1,c,6,n,1,c,2,(=O),x,n,3,c,4,(=O),x,Ring,Ring1
cytosine root root
n,1|prefhydro,Ring,Ring1,c,2,(=O),x,n,3,c,4,(N),n,c,5,c,6,Ring,Ring1
isocytosine root root
n,1|prefhydro,Ring,Ring1,c,2,(N),x,n,3,c,4,(=O),n,c,5,c,6,Ring,Ring1
guanine pseudosugar unknown x,x
guanine root root
n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,(N),n,N,1,c,6,(=O),x,c,5
,Ring,Ring1,Ring,Ring2
xanthine root root
n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,(=O),x,n,1,c,6,(=O),x,c,
5,Ring,Ring1,Ring,Ring2
hypoxanthine root root
n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,n,1,c,6,(O),x,c,5,Ring,R
ing1,Ring,Ring2
theophylline|theophyllin|aminophylline|aminophyllin root root
n,7,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,(C),x,c,2,(=O),x,n,1,(C),x,c,6,(=O),x,
c,5,Ring,Ring1,Ring,Ring2
theobromine|theobromin root root
n,7,Ring,Ring1,(C),x,c,8,n,9,c,4,Ring,Ring2,n,3,(C),x,c,2,(=O),x,n,1,c,6,(=O),x,
c,5,Ring,Ring1,Ring,Ring2
xanthopterin root root Oc1nc(N)nc2c1nc(O)cn2,x
isoxanthopterin root root O=C1C(N=CC2=O)=C(N2)NC(N)=N1,x
xanthopterid root root
n,1,Ring,Ring1,c,2,(N),x,n,3,c,4,(O),x,c,4a,Ring,Ring2,n,5,c,6,(O),x,c,7,n,8,c,8
a,Ring,Ring1,Ring,Ring2
pterin|pterine root root
n,1,Ring,Ring1,c,2,(N),x,N,3,C,4,(=O),x,c,4a,Ring,Ring2,n,5,c,6,c,7,n,8,c,8a,Rin
g,Ring2,Ring,Ring1
aminopterin root root
O,1@x,C(CCC(C(O)=O)NC(C3=CC=C(C=C3)NCC1=CN=C2C(C(N)=NC(N)=N2)=N1)=O)=O,x
vitaminh root root O=C(N2)NC1C2CS[C@H]1CCCCC(O)=O,x
brucine root root
O=C(C5)N(C4[C@@]2(CC7)[C@](N7C6)([H])C[C@@]3([H])C6=CCOC5[C@]34[H])C1=C2C=C(OC)C
(OC)=C1,x
struchnine root root
O=C(C5)N(C4[C@@]2(CC7)[C@](N7C6)([H])C[C@@]3([H])C6=CCOC5[C@]34[H])C1=C2C=,x,C,1
0,C,11,=C1,x
penicillan root root
C,x,[C@@H],3,Ring,Ring2,N,4,Ring,Ring1,C,5,(,x,[C@H],6,([H]),x,[C@@],6a,Ring,Rin
g1,([H]),x,S,1,C,2,Ring,Ring2,(C)C)=O,x

cephalosporan root root
C,x,C,4,Ring,Ring1,=,x,C,3,(COC(C)=O),x,C,2,S,1,[C@@],7a,(,x,[C@H],7,Ring,Ring2,
[H],x,),x,([H]),x,N,5,Ring,Ring1,C,6,Ring,Ring2,=O,x
vitaminb1|thiamine|thiamin|thiaminechloride|thiaminchlorid root root
O3.NC1=C(C[N+]2=CSC(CC3)=C2C)C=NC(C)=N1.[Cl-],x
vitaminb1nitrate|thiaminenitrate|thiaminnitrate root root
O3.NC1=C(C[N+]2=CSC(CC3)=C2C)C=NC(C)=N1.[O-][N+]([O-])=O,x
thiaminedisulfide root root
CC(N(C=O)CC1=CN=C(N=C1N)C)=C(SSC(CCO)=C(N(C=O)CC2=C(N)N=C(C)N=C2)C)CCO,x
vitaminb2|riboflavin root root
CC1=CC2=C(N=C(C(N3)=O)C(N2C[C@@H](O)[C@@H](O)[C@@H](O),x,C,5',O)=NC3=O)C=C1C,x
vitamine|alphatocopherol|atocopherol root root
CC1=C2C(O[C@@](CCC[C@H](C)CCC[C@H](C)CCC[C@H](C)C)(C)CC2)=C(C)C(C)=C1O,x
phenolsulfonphthalein|phenolsulfonephthalein root root
C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',c,4',(,x,O,x,),x,c,5',c,6',Ri
ng,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',c,4'',(,x,O,x,),x,c,5'',c,6'',Ring,Rin
g4
mcresolsulfonphthalein|mcresolsulfonephthalein root root
C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(O),x,c,3',c,4',(,x,C,x,),x,c,5',c
,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(O),x,c,3'',c,4'',(,x,C,x,),x,c,5'',c,
6'',Ring,Ring4
ocresolsulfonphthalein|ocresolsulfonephthalein root root
C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(,x,C,x,),x,c,5',c
,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',(O),x,c,4'',(,x,C,x,),x,c,5'',c,
6'',Ring,Ring4
pyrocatecholsulfonphthalein|pyrocatecholsulfonephthalein root root
C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(,x,O,x,),x,c,5',c
,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',(O),x,c,4'',(,x,O,x,),x,c,5'',c,
6'',Ring,Ring4
pyrogallolsulfonphthalein|pyrogallolsulfonephthalein root root
C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(,x,O,x,),x,c,3',(O),x,c,4',(,x,O,
x,),x,c,5',c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(,x,O,x,),x,c,3'',(O),x,c,
4'',(,x,O,x,),x,c,5'',c,6'',Ring,Ring4
thymolsulfonphthalein|thymolsulfonephthalein root root
C,1,Ring,Ring1,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(,x,C(C)C,x,),x,c,3',c,4',(,x,O,x,
),x,c,5',(C),x,c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(,x,C(C)C,x,),x,c,3'',
c,4'',(,x,O,x,),x,c,5'',(C),x,c,6'',Ring,Ring4
phenolphthalein root root
C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',c,4',(,x,O,x,),x,c,5',c,6',Ring,R
ing3,),x,c,1'',Ring,Ring4,c,2'',c,3'',c,4'',(,x,O,x,),x,c,5'',c,6'',Ring,Ring4
mcresolphthalein root root
C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(O),x,c,3',c,4',(,x,C,x,),x,c,5',c,6',
Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(O),x,c,3'',c,4'',(,x,C,x,),x,c,5'',c,6'',
Ring,Ring4
ocresolphthalein root root
C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(,x,C,x,),x,c,5',c,6',
Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',(O),x,c,4'',(,x,C,x,),x,c,5'',c,6'',
Ring,Ring4

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pyrocatecholphthalein root root
C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(O),x,c,4',(,x,O,x,),x,c,5',c,6',
Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',(O),x,c,4'',(,x,O,x,),x,c,5'',c,6'',
Ring,Ring4
pyrogallolphthalein root root
C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(,x,O,x,),x,c,3',(O),x,c,4',(,x,O,x,),
x,c,5',c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(,x,O,x,),x,c,3'',(O),x,c,4'',
(,x,O,x,),x,c,5'',c,6'',Ring,Ring4
thymolphthalein root root
C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(,x,C(C)C,x,),x,c,3',c,4',(,x,O,x,),x,
c,5',(C),x,c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(,x,C(C)C,x,),x,c,3'',c,4'
',(,x,O,x,),x,c,5'',(C),x,c,6'',Ring,Ring4
tetraiodophthalein|iodophthalein|iodophene|iodotetragnost root root
C,1,Ring,Ring1,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,(I),x,c,5,(I),x,c,6,(I),x,
c,7,(I),x,c,7a,Ring,Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',c,4',(,x,
O,x,),x,c,5',c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',c,4'',(,x,O,x,),x,
c,5'',c,6'',Ring,Ring4
fluorescein root root
C,1,Ring,Ring1,Ring,Ring5,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7
a,Ring,Ring2,Ring,Ring1,),x,c,10a,Ring,Ring3,c,1',c,2',c,3',(,x,O,x,),x,c,4',c,4
a',Ring,Ring3,O,x,c,5b',Ring,Ring4,c,5',c,6',(,x,O,x,),x,c,7',c,8',c,8a',Ring,Ri
ng5,Ring,Ring4
sulfonfluorescein root root
C,1,Ring,Ring1,Ring,Ring5,(,x,O,2,S,3,(=O)(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7
,c,7a,Ring,Ring2,Ring,Ring1,),x,c,10a,Ring,Ring3,c,1',c,2',c,3',(,x,O,x,),x,c,4'
,c,4a',Ring,Ring3,O,x,c,5b',Ring,Ring4,c,5',c,6',(,x,O,x,),x,c,7',c,8',c,8a',Rin
g,Ring5,Ring,Ring4
fluoran|fluorane root root
C,1,Ring,Ring1,Ring,Ring5,(,x,O,2,C,3,(=O),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7
a,Ring,Ring2,Ring,Ring1,),x,c,10a,Ring,Ring3,c,1',c,2',c,3',c,4',c,4a',Ring,Ring
3,O,x,c,5b',Ring,Ring4,c,5',c,6',c,7',c,8',c,8a',Ring,Ring5,Ring,Ring4
uramil root root N,n,C1C(=O)NC(=O)NC(=O)1,x
isosorbide root root
O,x,[C@H],2,Ring,Ring1,C,1,O,x,[C@@],4,Ring,Ring2,(,x,[H],x,),x,[C@],3,Ring,Ring
1,(,x,[H],x,),x,O,x,C,6,[C@H],5,Ring,Ring2,O,x
isoproterenol|isoprenaline root root CC(NCC(C1=CC(O)=C(O)C=C1)O)C,x
shikonin root root CC(C)=CC[C@@H](O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
alkannin root root CC(C)=CC[C@H](O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
shikalkin root root CC(C)=CCC(O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O,x
hyoscyamine root root CN1C2CCC1C[C@H](OC(C(CO)c3ccccc3)=O)C2,x
44'carbocyanine|cryptocyanine|kryptocyanine root root
[n+],1,Ring,Ring1,c,2,c,3,c,4,(,x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
2,Ring,Ring1,),x,C=CC=,x,C,4',Ring,Ring3,C,3',=,x,C,2',N,1',c,8a',Ring,Ring4,c,8
',c,7',c,6',c,5',c,4a',Ring,Ring4,Ring,Ring3
22'carbocyanine|pinacyanol root root
[n+],1,Ring,Ring1,c,2,(,x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
2,Ring,Ring1,),x,C=CC=,x,C,2',(,x,C,3',=,x,C,4',Ring,Ring3,),x,N,1',c,8a',Ring,R
ing4,c,8',c,7',c,6',c,5',c,4a',Ring,Ring4,Ring,Ring3
oxacarbocyanine root root
o,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5
',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
oxadicarbocyanine root root
o,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri

ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
oxatricarbocyanine root root
o,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
thiacyanine root root
s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c
,7a',Ring,Ring4,S,1',Ring,Ring3
thiacarbocyanine root root
s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5
',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
thiadicarbocyanine root root
s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
thiatricarbocyanine root root
s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
selenacarbocyanine root root
[se],1,Ring,Ring1,cC,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4'
,c,5',c,6',c,7',c,7a',Ring,Ring4,[Se],1',Ring,Ring3
hordenine root root CN(C)CCC1=CC=C(O)C=C1,x
maltol root root o1ccc(=O)c(O)c(C)1,x
coman root root Cc1=cc(=O)cco1,x
chrysoidine root root
c,4|p|para,(,x,c,3|m|meta,c,2|o|ortho,Ring,Ring1,),x,c,5,c,6,c,1,Ring,Ring1,N=Nc
2c(N)cc(N)cc2,x
alphafuril root root O=C(C1=CC=CO1)C(C2=CC=CO2)=O,x
anisil root root O=C(C1=CC=C(OC)C=C1)C(C2=CC=C(OC)C=C2)=O,x
alphaphellandrene root root CC1=CCC(C(C)C)C=C1,x
betaphellandrene root root CC(C(C=C1)CCC1=C)C,x
scopolamine|scopolamin root root C[N+]1([O-
])C2CCC1CC(OC(C(CO)C3=CC=CC=C3)=O)C2,x
pilocarpine|pilocarpin root root CC[C@H]1[C@@H](CC2=CN=CN2C)COC1=O,x
guanethidine root root NC(NCCN1CCCCCCC1)=N,x
lobeline root root CN1C(CC(C3=CC=CC=C3)O)CCCC1CC(C2=CC=CC=C2)=O,x
mercaptur root root C[C@H](CS)NC(C)=O,x
phenylmercaptur root root C[C@H](CSc1ccccc1)NC(C)=O,x
alphalip|alip root root CCCCCC1SSCC1,x
perill|perilla root root CC1=CCC(C(C)=C)CC1,x
biotin root root O,1@x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
biotinyl root root C,4@x,(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
biotinamide|biotinamid root root
N,x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
bisphenola root root
O1.Oc,4,Ring,Ring2,c,5,c,6,c,1,(,x,c,2,c,3,Ring,Ring2,),x,C(C)(C),x,c,1',Ring,Ri
ng3,c,2',c,3',c,4',Ring,Ring1,c,5',c,6',Ring,Ring3
pantothen root root CCCNC(C(C(CO)(C)C)O)=O,x
alloxan root root
N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,(=O),x,C,5,(=O),x,C,6,(=O),x,Ring,Ring1
croman root root Cc1occc(=O)c1,x

cinchon root root
C,9,(,x,c,4',Ring,Ring2,c,4a',(,x,c,5',c,6',c,7',c,8',Ring,Ring4,),x,c,8a',Ring,
Ring4,n,1'|a-1,c,2'|a-b,c,3'|a-
t,Ring,Ring2,),x,C,8,Ring,Ring1,N(CC3)CC(,x,C,10,=,x,C,11,)C3C1,x
1011dihydrocinchon root root
C,9,(,x,c,4',Ring,Ring2,c,4a',(,x,c,5',c,6',c,7',c,8',Ring,Ring4,),x,c,8a',Ring,
Ring4,n,1'|a-1,c,2'|a-b,c,3'|a-
t,Ring,Ring2,),x,C,8,Ring,Ring1,N(CC3)CC(,x,C,10,C,11,)C3C1,x
cinchonine|cinchonin root root
O[C@@H]([C@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
1011dihydrocinchonine|1011dihydrocinchonin root root
O[C@@H]([C@H]2N(CC4)C[C@@H](CC)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
quinidine root root
O[C@@H]([C@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
1011dihydroquinidine root root
O[C@@H]([C@H]2N(CC4)C[C@@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
cinchonidine|cinchonidin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
1011dihydrocinchonidine|1011dihydrocinchonidin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1,x
quinine|quinin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
1011dihydroquinine|1011dihydroquinin|dihydroquinine|dihydroquinin|hydroquinine|h
ydroquinin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
hepes root root S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o,),x,CCN(CC1)CCN1CCO,x
pipes root root O=S(CCN1CCN(CCS(=O)(O)=O)CC1)(O)=O,x
popop root root C1(C2=CC=C(C4=NC=C(C5=CC=CC=C5)O4)C=C2)=NC=C(C3=CC=CC=C3)O1,x
dibenzosuber root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,C,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,C,10,C,11,c,11a,Ring,Ring2,Ring,Ring1
benzosuber root root
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,c,5a,Ring,Ring2,c,6,c,7,c,8,c,9,c,9a,Ring,Ring2,R
ing,Ring1
orthosilicate root root
[Si],x,(,x,O,1@o''',),x,(,x,O,1@o'',),x,(,x,O,1@o',),x,O,1@o
orthotitanate root root
[Ti],x,(,x,O,1@o''',),x,(,x,O,1@o'',),x,(,x,O,1@o',),x,O,1@o
gona|gon root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,C,17,C,13,Ring,Ring4,C,12,C,11,C,9,Ring,Ring3,C,10,Ring,Ring1
,Ring,Ring2
estra|oestra|estr|oestr root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C,9,Ring,Ring3
,C,10,Ring,Ring1,Ring,Ring2
equilen root steroid
c,3,(O)(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,c,6,c,7,c,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,c,9,
Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
dihydroequilen root steroid
c,3,(O)(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,c,6,c,7,c,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,C,17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,c,9,R
ing,Ring3,c,10,Ring,Ring1,Ring,Ring2
androsta|androst|etiochola|etiochol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri

ng,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring
3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
etioallochola|etioallochol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
etien root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(C),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
etian root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(C),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,
Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
androstenediol root steroid
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,C,8,Ring
,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@H],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x
,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
androstenedione root steroid
C,3,(=O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ri
ng3,C,14,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,
C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
pregna|pregn root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,
12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
allopregna|allopregn root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,),x,[C@@],13,Ring,Ring4,(,x
,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
chola|chol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21,),x,[C@@],1
3,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring
2,C,19
cholesta|cholest|coprost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,2
7,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],1
0,Ring,Ring1,Ring,Ring2,C,19
lanosta|lanost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,[C@],4,(,x,C,28,)(,x,C,29,),x,C,5,Ring,Ring2,C,6,
C,7,C,8,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,30,),x,C,15,C,16,[C@],17,(,x,[C@@],2
0,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x
,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
dammara|dammar root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,[C@],4,(,x,C,28,)(,x,C,29,),x,C,5,Ring,Ring2,C,6,
C,7,C,8,Ring,Ring3,[C@@],14,Ring,Ring4,(,x,C,30,),x,C,15,C,16,[C@],17,(,x,[C@@],
20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,C,
12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
urs root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,x,)(,x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[
C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(C),27,C,x,C,x,[C@@],x,Ring,Ring5,(C),
28,C,22,C,21,[C@@H],20,(,x,C,30,),x,[C@H],19,(,x,C,29,),x,[C@@],18,([H]),x,Ring,
Ring5,[C@@],13,Ring,Ring4,(,x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,R
ing1,Ring,Ring2,C,x

lup root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,x,)(,x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[
C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(C),27,C,x,C,x,[C@@],x,Ring,Ring5,(C),
28,C,22,C,21,[C@@H],19,(,x,C,20,(,x,C,29,),x,C,30,),x,[C@@],18,([H]),x,Ring,Ring
5,[C@@],13,Ring,Ring4,(,x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,x
taraxaster root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,x,)(,x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[
C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,),x,C,x,C,x,[C@@],x,Ring,Ring5
,(C),28,C,22,C,21,C,20,(=,x,C,30,),x,C,19,(,x,C,29,),x,[C@],18,([H]),x,Ring,Ring
5,[C@@],13,Ring,Ring4,(,x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,x
oleane|olean root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,23,)(,x,C,24,),x,C,5,Ring,Ring2,C,6,C,7
,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,),x,C,15,C,16,[C@@],x,Ring,R
ing5,(C),28,C,22,C,21,C,20,(,x,C,30,)(,x,C,29,),x,C,x,[C@@],18,([H]),x,Ring,Ring
5,[C@@],13,Ring,Ring4,(,x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,19
olean loveracid steroid
C,x,Ring,Ring6,.,.,x,C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,23,)(,x,C,24,),x,C,5
,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,),x,C,15,
C,16,[C@@],x,Ring,Ring5,Ring,Ring6,C,x,C,x,C,x,(,x,C,x,)(,x,C,29,),x,C,x,[C@],x,
([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,=,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Rin
g,Ring1,Ring,Ring2,C,19
olean|oleanol loveracid steroid
C,x,Ring,Ring6,.,.,x,[C@H],3,(O)(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,23,)(,x,C,24,
),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,),
x,C,15,C,16,[C@@],x,Ring,Ring5,Ring,Ring6,C,x,C,x,C,x,(,x,C,x,)(,x,C,29,),x,C,x,
[C@],x,([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,=,x,C,12,C,11,C,9,Ring,Ring3,[C@@]
,10,Ring,Ring1,Ring,Ring2,C,19
glycyrrhetin root steroid
C,29,Ring,Ring6,.,.,x,[C@],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,x,)(,x,C,x
,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,)
,x,C,x,C,x,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,[C@],20,(,x,C,30,),x,Ring,Ring6,C
,x,[C@@],18,([H]),x,Ring,Ring5,C,13,Ring,Ring4,=,x,C,12,C,11,(=O),x,C,9,Ring,Rin
g3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
glycyrrhet root steroid
C,29,Ring,Ring6,.,.,x,[C@],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,x,)(,x,C,x
,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,)
,x,C,x,C,x,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,[C@],20,(,x,C,30,),x,Ring,Ring6,C
,x,[C@@],18,([H]),x,Ring,Ring5,C,13,Ring,Ring4,=,x,C,12,C,11,(=O),x,C,9,Ring,Rin
g3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
solanid root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,[C@],8,([H]),x,Ring,Ri
ng3,[C@@],14,([H]),x,Ring,Ring4,C,15,[C@@],16,([H]),x,Ring,Ring5,N,28,Ring,Ring6
,C,x,[C@@],25,(C),x,C,24,C,23,[C@@],22,([H]),x,Ring,Ring6,[C@@],x,(C),x,[C@@],x,
([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,(C),18,C,12,C,11,C,9,Ring,Ring3,[C@@],10,
Ring,Ring1,Ring,Ring2,C,x
cholester root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,c,5,Ring,Ring2,c,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,
27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],
10,Ring,Ring1,Ring,Ring2,C,19
lanoster root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,28,)(,x,C,29,),x,C,5,Ring,Ring2,=,x,C,6
,C,7,C,8,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,30,),x,C,15,C,16,[C@],17,(,x,[C@@H]

,20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(
,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
ergosta|ergost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(C),x,C,25,(,x,C,
26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Rin
g3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
campesta|campest root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@@H],24,(C),x,C,25,(,x,C
,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ri
ng3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
poriferasta|poriferast root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(CC),x,C,25,(,x,C
,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ri
ng3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
stigmasta|stigmast root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@@H],24,(,x,C,28,C,29,),
x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11
,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
pregnenolone root steroid
C,1,Ring,Ring1,C,2,C,3,(O),x,C,4,c,5,Ring,Ring2,c,6,C,7,C,8,Ring,Ring3,C,14,Ring
,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,)
,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
prednisolone|prednisolon root steroid
C,1,Ring,Ring1,=,x,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,
C,14,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@
],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,(,x,O,x,),x,C,9,Ring,Ring3,[C@@],10,Ring,
Ring1,Ring,Ring2,C,19
progesterone|progesteron root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin
g,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,
),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
tetrahydroprogesterone|tetrahydroprogesteron root steroid
C,1,Ring,Ring1,C,2,C,3,(O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring
,Ring4,C,15,C,16,[C@],17,(,x,C,20,(O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),
x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
hydrocortisone|hydrocortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13
,Ring,Ring4,(,x,C,18,),x,C,12,[C@@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,19
dihydrocortisone|dihydrocortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin
g,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13,Rin
g,Ring4,(,x,C,18,),x,C,12,[C@@H],11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ri
ng,Ring2,C,19
tetrahydrocortisone|tetrahydrocortison root steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13
,Ring,Ring4,(,x,C,18,),x,C,12,[C@@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,19
cortisone|cortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=O),x,C,21,O,x,),x,(,x,O,x,),x,[C@@],13

,Ring,Ring4,(,x,C,18,),x,C,12,[C@@H],11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring
1,Ring,Ring2,C,19
androsterone root steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9
,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
isoandrosterone root steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,
Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,
Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
aldosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,1
8,=O,x,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,1
9
pregnanolone root steroid
C,3,(O)(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C
,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
testosteron|testosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
dihydrotestosteron|dihydrotestosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
oestradiol|estradiol|betaoestradiol|betaestradiol root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11
,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
oestriol|estriol root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,[C@@],16,(O),x,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x
,C,12,C,11,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
oestrone|estrone root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C
,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
brassinolid|brassinolide root steroid
[C@@H],3,(O),x,(,x,[C@H],2,(O),x,C,1,Ring,Ring1,),x,C,4,[C@],5,Ring,Ring2,([H]),
x,C,6,(=O)O,x,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,
(,x,[C@H],22,(O),x,[C@H],23,(O),x,[C@@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,2
1,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
ng1,Ring,Ring2,C,19
calcidiol root root
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C,2
5,(,x,C,26,)(O),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
,9,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
calciol|cholecalciferol|vitamind3 root root
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8|
a-
r,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C
,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11|a-
t,C,9|a-b,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19

70

calcitriol root root
[C@H],3,(O),x,(,x,C,2,[C@H],1,(O),x,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,
7,=,x,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,2
3,C,24,C,25,(,x,C,26,)(O),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C
,12,C,11,C,9,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
corticosterone root steroid
C,3,(=O)(,x,C,2,C,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,O,x,),x,[C@@],13,Ring,Ring4,
(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C
,19
cortisol root steroid
C,3,(=O)(,x,C,2,C,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,O,x,)(O),x,[C@@],13,Ring,Rin
g4,(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring
2,C,19
ecdysone root steroid
[C@H],3,(O),x,(,x,[C@@H],2,(O),x,C,1,Ring,Ring1,),x,C,4,[C@@],5,Ring,Ring2,([H])
,x,C,6,(=O),x,C,7,=,x,C,8,Ring,Ring3,[C@],14,Ring,Ring4,(O),x,C,15,C,16,[C@],17,
(,x,[C@@],20,(,x,C,22,(O),x,C,23,C,24,C,25,(O)(,x,C,26,),x,C,27,),x,C,21,),x,[C@
@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,
Ring2,C,19
ercalciol|ergocalciferol root root
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,=,x,C,23,[C@H
],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,
C,12,C,11,C,9,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
ergosterol root steroid
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,=,x,C,23,[C@H
],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,
C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
lumisterol root steroid
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,=,x,C,23,[C@H
],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,
C,12,C,11,[C@],9,([H]),x,Ring,Ring3,[C@],10,Ring,Ring1,Ring,Ring2,C,19
cardanolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,Ring,Ring5,C,21,O,x,C,23,(=O),x,C,22,Rin
g,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,R
ing,Ring1,Ring,Ring2,C,19
card2022enolide|2022cardenolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,C,20,Ring,Ring5,C,21,O,x,C,23,(=O),x,C,22,=,x,Rin
g,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,R
ing,Ring1,Ring,Ring2,C,19
digitoxigenin root steroid
O,x,[C@@],3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@],5,Ring,Ring2,([H]),x,C,6,C,7,C,
8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,Ring,Ring5,C,21,O,x,C,23
,(=O),x,C,22,=,x,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,R
ing,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
bufanolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,Ring,Ring5,C,21,O,x,C,24,(=O),x,C,23,C,2
2,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@]
,10,Ring,Ring1,Ring,Ring2,C,19

bufadienolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,Ring,Ring5,=,x,C,21,O,x,C,24,(=O),x,C,23
,=,x,C,22,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Rin
g3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
cev root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,[C@@],1
4,([H]),x,Ring,Ring4,C,15,C,16,[C@@],17,([H]),x,Ring,Ring5,[C@@H],20,(C),x,[C@@]
,x,([H]),x,Ring,Ring6,C,x,C,x,[C@H],x,(C),x,C,x,N,x,Ring,Ring6,C,x,[C@],x,([H]),
x,Ring,Ring5,[C@@],12,([H]),x,Ring,Ring4,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,19
solidan root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,Ring,Ring5,[C@],17,([H])(,x,[C@],20,(,x,C,21,),x,[C@],22,([H]
),x,Ring,Ring6,C,23,C,24,[C@H],25,(,x,C,27,),x,C,26,N,28,Ring,Ring6,Ring,Ring5,)
,x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,19
spirost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,[C@],16,([H])(,x,O,x,Ring,Ring5,),x,[C@],17,([H])(,x,[C@@],20,(,x,
[C@@],22,Ring,Ring5,(,x,O,x,Ring,Ring6,),x,C,23,C,24,C,25,(,x,C,26,Ring,Ring6,),
x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C
@@],10,Ring,Ring1,Ring,Ring2,C,19
spirosol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,[C@],16,([H])(,x,O,x,Ring,Ring5,),x,[C@],17,([H])(,x,[C@],20,(,x,C
,22,Ring,Ring5,(,x,N,x,Ring,Ring6,),x,C,23,C,24,C,25,(,x,C,26,Ring,Ring6,),x,C,2
7,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],1
0,Ring,Ring1,Ring,Ring2,C,19
tomatid root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@H],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,
Ring3,C,14,Ring,Ring4,C,15,[C@],16,([H])(,x,O,x,Ring,Ring5,),x,[C@],17,([H])(,x,
[C@],20,(,x,[C@],22,Ring,Ring5,(,x,N,x,Ring,Ring6,),x,C,23,C,24,[C@@H],25,(,x,C,
26,Ring,Ring6,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
solasod root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@H],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,
Ring3,C,14,Ring,Ring4,C,15,[C@],16,([H])(,x,O,x,Ring,Ring5,),x,[C@],17,([H])(,x,
[C@],20,(,x,[C@@],22,Ring,Ring5,(,x,N,x,Ring,Ring6,),x,C,23,C,24,[C@H],25,(,x,C,
26,Ring,Ring6,),x,C,27,),x,C,21,),x,[C@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
furost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,[C@],16,([H])(,x,O,x,Ring,Ring5,),x,[C@],17,([H])(,x,[C@@],20,(,x,
[C@],22,Ring,Ring5,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,R
ing4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
chol loveracid steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@@H],7,(O),x,C,8,Ring,
Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,2
1,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,[C@@H],12,(O),x,C,11,C,9,Ring,Ring3,[C@@]
,10,Ring,Ring1,Ring,Ring2,C,19
lithochol loveracid steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21,),x,[C@@
],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,R
ing2,C,19

dehydrochol loveracid steroid
C,1,Ring,Ring1,C,2,C,3,(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,(=O),x,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21,),x,[
C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,(=O),x,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
ng1,Ring,Ring2,C,19
hyodeoxychol loveracid steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,[C@@H],6,(O),x,C,7,C,8,Ring
,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,
21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,R
ing1,Ring,Ring2,C,19
chenodeoxychol loveracid steroid
C,1,Ring,Ring1,C,2,C,3,[C@@H],4,(O),x,C,5,Ring,Ring2,C,6,[C@@H],7,(O),x,C,8,Ring
,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,
21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,R
ing1,Ring,Ring2,C,19
ursodeoxychol loveracid steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@H],7,(O),x,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21
,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Rin
g1,Ring,Ring2,C,19
tauroursodeoxychol loveracid steroid
S,x,(=O),x,(=O),x,(,x,O,1@x,),x,C,x,C,x,N,x,Ring,Ring5,.,.,x,C,1,Ring,Ring1,C,2,[C
@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@H],7,(O),x,C,8,Ring,Ring3,C,14,Ring,Ring4
,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=O),x,Ring,Ring5,),x,C,21,)
,x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,
Ring,Ring2,C,19
taurochol loveracid steroid
S,x,(=O),x,(=O),x,(,x,O,1@x,),x,C,x,C,x,N,x,Ring,Ring5,.,.,x,C,1,Ring,Ring1,C,2,C,
3,[C@H],4,(O),x,C,5,Ring,Ring2,C,6,[C@@H],7,(O),x,C,8,Ring,Ring3,C,14,Ring,Ring4
,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=O),x,Ring,Ring5,),x,C,21,)
,x,[C@@],13,Ring,Ring4,(,x,C,x,),x,[C@@H],12,(O),x,C,11,C,9,Ring,Ring3,[C@@],10,
Ring,Ring1,Ring,Ring2,C,19
glycochol loveracid steroid
C,1,Ring,Ring1,C,2,C,3,[C@H],4,(O),x,C,5,Ring,Ring2,[C@@H],6,(O),x,C,7,C,8,Ring,
Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=O)NCC
,x,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,[C@@H],12,(O),x,C,11,C,9,Ring,R
ing3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
oxymetholone root steroid
C,3,(=O)(,x,C,2,(=CO),x,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(O)(C),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,
C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
homo natderiver nathomo x,x
nor natderiver natnor x,x
seco natderiver natseco x,x
abeo natderiver natabeo x,x
cyclo natderiver cyclo x,x
rightarrow|arrow|fwdarrow|fwdarw unknown natarrow x,x
flophemesyl root root [Si],4@x,(C)(C)c1c(F)c(F)c(F)c(F)c(F)1,x
diethylenetriamine root root N,n|1,C,2,C,3,N,n''|4,C,5,C,6,N,n'|7
triethylenetetramine root root N,n,CC,x,N,n'',CC,x,N,n''',CC,x,N,n'
tetraethylenepentamine root root
N,n,CC,x,N,n'',CC,x,N,n''',CC,x,N,n'''',CC,x,N,n'
pentaethylenehexamine root root
N,n,CC,x,N,n'',CC,x,N,n''',CC,x,N,n'''',CC,x,N,n''''',CC,x,N,n'
cupferron root root O=NN([O-])c1ccccc1.[NH4+],x
camphene root root C=C(CC(CC2)C1(C)C)C12C,x

isopinocamphe root root
C,3,Ring,Ring1,C,4,C,5,(,x,C,6,Ring,Ring2,),x,C,7,(C)(C),x,C,1,Ring,Ring2,C,2,(C
),x,Ring,Ring1
choline root root O,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
phosphocholine root root O,1@x,P,x,(=O),x,([O-
]),x,O,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
diphosphocholine root root O,1@x,P,x,(=O),x,(,x,O,1@x,),x,O,x,P,x,(=O),x,([O-
]),x,O,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
phosphoethanolamine root root O,1@x,P,x,(=O),x,(O),x,O,x,C,b|beta,C,a|alpha,N,x
fluorocholine root root F,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
chlorocholine root root Cl,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
bromocholine root root Br,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
iodocholine root root I,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
betaine|betain root root [O-],x,C,x,(=O),x,C,a|alpha,[N+](C)(C)C,x
betainealdehyde|betainaldehyd root root [H],x,C,x,(=O),x,C,a|alpha,[N+](C)(C)C,x
carnitine|carnitin root root O,1@o,Ring,Ring1,.,x,[O-
],x,C,x,(=O),x,C,a|alpha,C,b|beta,Ring,Ring1,C,g|gamma,[N+](C)(C)C,x
carnitinamide root root
N,x,C,x,(=O),x,C,a|alpha,C,b|beta,(O),1@o,C,g|gamma,[N+](C)(C)C,x
aminocarnitine|aminocarnitin root root [O-
],x,C,x,(=O),x,C,a|alpha,C,b|beta,(N),x,C,g|gamma,[N+](C)(C)C,x
exact-azine root root n1ccccc1,x
exact-ether root root CCOCC,x
exact-alcohol root root OCC,x
exact-salt root root [Na+].[Cl-],x
exact-sulfur root root S1SSSSSSS1,x
exact-phenazo root root OC(C=C4)=CC=C4N=NC(C([N+]([O-
])=O)=C2)=CC=C2C1=CC([N+]([O-])=O)=C(N=NC3=CC=C(O)C=C3)C=C1,x
exact-nitron root root C2([N-]N(C4=CC=CC=C4)C=[N+]2C3=CC=CC=C3)=NC1=CC=CC=C1,x
exact-anthranil root root c1onc2ccccc12,x
exact-acetal root root CC(OCC)OCC,x
exact-sugar root root
OC[C@@]1([C@@H](O)[C@H](O)[C@H](O1)CO)O[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO
)O2,x
exact-bisacrylamide root root O=C(C=C)NCNC(C=C)=O,x
exact-dopa root root
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,c,x,Ring,Ring2,c,
2|o|ortho,c,3|m|meta,(O),x,c,4|p|para,(O),x,c,5,c,6,Ring,Ring2
exact-hydrogen root root [H][H],x
exact-deuterium root root [2H][2H],x

zincon root root
O[S](=O)(C1=CC(N=NC(C3=CC=CC=C3)=NNC2=CC=CC=C2C(O)=O)=C(O)C=C1)=O,x
chloroform root chloroform C([H])(Cl)(Cl)Cl,x
fluoroform root chloroform C([H])(F)(F)F,x
bromoform root chloroform C([H])(Br)(Br)Br,x
iodoform root chloroform C([H])(I)(I)I,x
ferricyanide root root [Fe-3](C#N)(C#N)(C#N)(C#N)(C#N)(C#N),x
ferrocyanide root root [Fe-4](C#N)(C#N)(C#N)(C#N)(C#N)(C#N),x
dibromochloride root root [Cl-](Br)Br,x
dibromoiodide root root [I-](Br)Br,x
dichloroiodate|dichloroiodide root root [I-](Cl)Cl,x
diiodoaurate root root [Au-](I)I,x
dichloroaurate root root [Au-](Cl)Cl,x
dibromoaurate root root [Au-](Br)Br,x
bromodiiodide root root [Br-](I)I,x
dichlorobromide root root [Br-](Cl)Cl,x

tetrachloroiodate|iodotetrachloride root root [I-](Cl)(Cl)(Cl)Cl,x
chlorochromate root root [O-][Cr](=O)(=O)Cl,x
fluorochromate root root [O-][Cr](=O)(=O)F,x
fluoroborate|fluoroborat|tetrafluoroborate|tetrafluoroborate1|tetrafluoroborat|b
f4|borofluoride|borofluorid|fluoborate|fluoborat root root [B-](F)(F)(F)F,x
fluorosilicate|fluorosilicat|hexafluorosilicate|hexafluorosilicat root root [Si-
-](F)(F)(F)(F)(F)F,x
borohydride|borohydrid root root [B-],x
borodeuteride|borodeuterid root root [B-]([2H])([2H])([2H])[2H],x
cyanoborodeuteride|cyanoborodeuterid root root [B-]([2H])([2H])([2H])C#N,x
aluminohydride|aluminohydrid root root [Al-],x
persulfate|persulfat|peroxodisulfate|peroxodisulfat root root
O,1@x,S(=O)(=O)OOS(=O)(=O),x,O,1@x
bifluoride|bifluorid root root [F-],x,.[H]F,x
water root root [H]O[H],x
hydrofluoride root hydrochloride [H]F,x
hydrochloride|hcl root hydrochloride [H]Cl,x
2hcl root hydrochloride [H]Cl.[H]Cl,x
3hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl,x
4hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl.[H]Cl,x
5hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl.[H]Cl.[H]Cl,x
methochloride|chlormethylate root hydrochloride CCl,x
methobromide|brommethylate root hydrochloride CBr,x
hydrobromide|hbr root hydrochloride [H]Br,x
2hbr root hydrochloride [H]Br.[H]Br,x
3hbr root hydrochloride [H]Br.[H]Br.[H]Br,x
4hbr root hydrochloride [H]Br.[H]Br.[H]Br.[H]Br,x
5hbr root hydrochloride [H]Br.[H]Br.[H]Br.[H]Br.[H]Br,x
hydrotribromide|hbr root hydrochloride [H]Br(Br)Br,x
hydroiodide|hydriodide root hydrochloride [H]I,x
methoiodide|methiodide root hydrochloride CI,x
ethoiodide|ethiodide root hydrochloride CCI,x
hydrate|h2o root hydrochloride [H]O[H],x
deuterate|d2o root hydrochloride [2H]O[2H],x
etherate root hydrochloride
O(C([H])([H])C([H])([H])[H])C([H])([H])C([H])([H])[H],x
bitartarate|bitartrate|hydrogentartrate root hydrochloride
O,1@x,C,1,(=,x,O,x,),x,C,2,(,x,O,x,),x,C,3,(,x,O,x,),x,C,4,(=,x,O),x,O,x,[H],x
dbitartrate|hydrogendtartrate root hydrochloride
O,1@x,C,1,(=,x,O,x,),x,[C@@H],2,(,x,O,x,),x,[C@H],3,(,x,O,x,),x,C,4,(=,x,O),x,O,
x,[H],x
lbitartrate|hydrogenltartrate root hydrochloride
O,1@x,C,1,(=,x,O,x,),x,[C@H],2,(,x,O,x,),x,[C@@H],3,(,x,O,x,),x,C,4,(=,x,O),x,O,
x,[H],x
bimaleate|hydrogenmaleate root hydrochloride
O,1@x,C,1,(=,x,O,x,),x,/,x,C,2,=,x,C,3,\,x,C,4,(=,x,O),x,O,x,[H],x
bisuccinate|hydrogensuccinate root hydrochloride
O,1@x,C,1,(=,x,O,x,),x,C,2,C,3,C,4,(=O)O[H],x
biphthalate root hydrochloride
O,1@x,C(=O),x,c,1,Ring,Ring1,c,2,(C(=O)O[H]),x,c,3,c,4,c,5,c,6,Ring,Ring1
hydrogenoxalate root hydrochloride
O,1@x,C,1,(=,x,O,x,),x,C,2,(=,x,O),x,O,x,[H],x
bisulfate|bisulfat|hydrogensulfate root root O,1@x,S(=O)(=O)O[H],x
bisulfite|bisulfit|hydrogensulfite root root O,1@x,S(=O)O[H],x
bisulfide|bisulfid|hydrogensulfide root root S,1@x,[H],x
glycol|cellosolve|cellosolv root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,O,1@x,.,x,O,1@x,Ring,Ring1

thioglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,S,1@x,.,x,O,1@x,Ring,Ring1
dithioglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,S,1@x,.,x,S,1@x,Ring,Ring1
selenoglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Se],1@x,.,x,O,1@x,Ring,Ring1
diselenoglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Se],1@x,.,x,[Se],1@x,Ring,Ring1
telluroglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Te],1@x,.,x,O,1@x,Ring,Ring1
ditelluroglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Te],1@x,.,x,[Te],1@x,Ring,Ring1
tempo root root
C,4,Ring,Ring1,C,5,C,6,(C)(C),x,N,1,(,x,O,16@x,),x,C,2,(C)(C),x,C,3,Ring,Ring1
proxyl root root
C,3,Ring,Ring1,C,2,(C)(C),x,N,1,(,x,O,16@x,),x,C,5,(C)(C),x,C,4,Ring,Ring1
nitroxide|nitroxyl root root N,n,O,16@x
nitramine root root N,n,[N+](=O)[O-],x
nitramino root root N,4@n,[N+](=O)[O-],x
special-oxine root root
n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,(O),x,c,8a,Rin
g,Ring1,Ring,Ring2
special-azine|ketazine root azine N,8@x,N,8@x
oxime|oxim|antioxime root oxime N,8@x,O,o
hydrazone|hydrazon root oxime N,8@x,N,n
semicarbazone|semicarbazon root oxime N,8@1,N,2,C,3,(=,x,O,x,),x,N,4
azino root bridge N,8@x,N,8@x
azimino root bridge N,4@x,N,x,=,x,N,4@x
biimino|biimin root bridge N,4@x,N,4@x
epidioxy root bridge O,4@x,O,4@x
epidithio|epidithi root bridge S,4@x,S,4@x
epimino root bridge N,5@x
epithio root bridge S,5@x
episeleno root bridge [Se],5@x
epitelluro root bridge [Te],5@x
epithioximino|epithioximin root bridge S,4@x,O,x,N,4@x
epoxy root bridge O,5@x
epoxyimino|epoxyimin root bridge O,4@x,N,4@x
epoxynitrilo root bridge O,4@x,N,8@x
epoxythio|epoxythi root bridge O,4@x,S,4@x
epoxythioxy root bridge O,4@x,S,x,O,4@x
epitrithio|epitrithi root bridge S,4@x,S,x,S,4@x
cyanohydrin root oxime O,4@x,.,x,C,4@x,#N,x
fluorohydrin root oxime O,4@x,.,x,F,4@x
chlorohydrin root oxime O,4@x,.,x,Cl,4@x
bromohydrin root oxime O,4@x,.,x,Br,4@x
iodohydrin root oxime O,4@x,.,x,I,4@x
acetal|ketal|semiacetal|demiacetal|hemiacetal|semiketal|demiketal|hemiketal|glyc
olacetal|glycolketal root oxime O,4@x,.,x,O,4@x
mercaptal|mercaptole root oxime S,4@x,.,x,S,4@x
ketone|keton root ketone C,x,=,x,O,x
ketoxime root ketone C,x,=,x,N,x,O,x
ketoximino root ketone C,x,=,x,N,x,O,4@x
ketyl root ketone C,4@x,[O-],x
sulfoxide|sulfoxid root ketone S,x,=,x,O,x
sulfone|sulfon root ketone S,x,(=,x,O,x,),x,=,x,O,x
sulfimide|sulfimid|sulfilimine|sulfilimin root ketone S,x,=,x,N,x

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sulfoximide|sulfoximid|sulfoximine|sulfoximin root ketone
S,x,(=,x,O,x,),x,=,x,N,x
selenoxide|selenoxid root ketone [Se],x,=,x,O,x
selenone|selenon root ketone [Se],x,(=,x,O,x,),x,=,x,O,x
selenimide|selenimid root ketone [Se],x,=,x,N,x
selenoximide|selenoximid root ketone [Se],x,(=,x,O,x,),x,=,x,N,x
telluroxide|telluroxid root ketone [Te],x,=,x,O,x
tellurone|telluron root ketone [Te],x,(=,x,O,x,),x,=,x,O,x
tellurimide|tellurimid root ketone [Te],x,=,x,N,x
telluroximide|telluroximid root ketone [Te],x,(=,x,O,x,),x,=,x,N,x
peroxide|peroxid root ketone O,x,O,x
persulfide|persulfid root ketone S,x,S,x
formal root ketone O,x,Ring,Ring1,.,x,O,x,C,x,Ring,Ring1
ether root ether O,x
etherof root ofether O,x
thioether root ether S,x
selenoether root ether [Se],x
telluroether root ether [Te],x
oin oin unknown C,1@b|beta,(O),x,C,1@a|alpha,=O,x
ano methanomaker unknown x,x
quinone|quinon suffix quinone O,8@x
quinodimethane|quinodimethan suffix quinone C,10@x
radical radical unknown x,x
yl suffix yl 1,yl
ylidene|yliden|ilidene|iliden| suffix yl 2,yl
ylidyne|ylidyn|ilidyne|ilidyn suffix yl 3,yl
ane|an suffix ignore x,x
ine|in suffix ignore x,x
ene|en suffix bondchange 2,bond
yne|yn suffix bondchange 3,bond
thiol|ylthiol suffix suffix S,4@s
ol suffix olsuffix O,4@x
olate suffix suffix [O-],4@x
anethiolate|thiolato suffix suffix [S-],4@x
one|on suffix reqcarbon O,8@x
thione suffix reqcarbon S,8@x
selenone|selone suffix reqcarbon [Se],8@x
tellurone suffix reqcarbon [Te],8@x
imine root oxime N,8@n
imine imine suffix N,8@n
iminium root oxime [N+],8@x
iminium imine suffix [N+],8@x
glycol glycol unknown O,4@o,.,x,O,4@o'
thioglycol glycol unknown S,4@s,.,x,O,4@o
dithioglycol glycol unknown S,4@s,.,x,S,4@s'
selenoglycol glycol unknown [Se],4@x,.,x,O,4@x
diselenoglycol glycol unknown [Se],4@x,.,x,[Se],4@x
telluroglycol glycol unknown [Te],4@x,.,x,O,4@x
ditelluroglycol glycol unknown [Te],4@x,.,x,[Te],4@x
cyanohydrin glycol unknown C,4@x,#N,x,.,x,O,4@x
fluorohydrin glycol unknown F,4@x,.,x,O,4@x
chlorohydrin glycol unknown Cl,4@x,.,x,O,4@x
bromohydrin glycol unknown Br,4@x,.,x,O,4@x
iodohydrin glycol unknown I,4@x,.,x,O,4@x
oxide counterion oxide O,8@x
sulfide|mercaptide counterion oxide S,8@x
selenide counterion oxide [Se],8@x
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telluride counterion oxide [Te],8@x
methanoxymethano root methanobridge C,4@x,O,x,C,4@x
etheno root methanobridge C,4@x,=,x,C,4@x
metheno root metheno C,5@x
obenzeno root methanobridge c,4@x,Ring,Ring1,c,4@x,c,x,c,x,c,x,c,x,Ring,Ring1
epoxide|enoxide counterion bridge O,5@x
episulfide counterion bridge S,5@x
sultam counterion bridge S,4@x,(=,x,O,x,),x,(=,x,O,x,),x,N,4@x
sultone|sultone counterion bridge S,4@x,(=,x,O,x,),x,(=,x,O,x,),x,O,4@x
dicarboximide|dicarboxylicimide|dicarboxylicacidimide counterion bridge
C,4@x,(=,x,O,x,),x,N,x,C,4@x,=,x,O,x
dicarboximido counterion bridge
C,4@x,(=,x,O,x,),x,Ring,Ring1,.,x,C,4@x,Ring,Ring2,=,x,O,x,.,x,N,4@x,Ring,Ring1,
Ring,Ring2
carbolactam counterion bridge C,4@x,(=,x,O,x,),x,O,4@x
nitride counterion ionable N,12@x
phosphide counterion ionable P,12@x
antimonide counterion ionable [Sb],12@x
arsenide counterion ionable [As],12@x
hydroxide|hydroxid counterion ionable O,4@x
deuteroxide|deuteroxid counterion ionable O,4@x,[2H],x
hydrosulfide|hydrosulfid|sulfhydrate|sulfhydrat counterion ionable S,4@x
hydroselenide|hydroselenid counterion ionable [Se],4@x
hydrotelluride|hydrotellurid counterion ionable [Te],4@x
hydride|hydrid counterion ionable [H],4@1
deuteride|deuterid counterion ionable [2H],4@1
fluoride|fluorid counterion ionable F,4@1
chloride|chlorid|muriate counterion ionable Cl,4@1
bromide|bromid counterion ionable Br,4@1
iodide|iodid counterion ionable [I],4@1
acetylide counterion ionable C,4@x,#[C-],x
cyanide|cyanid counterion ionable C,4@x,#N,x
isocyanide|isocyanid|isonitrile counterion ionable [N+],4@x,#[C-],x
cyanate|cyanat counterion ionable O,4@x,C#N,x
isocyanate|isocyanat counterion ionable N,4@x,=C=O,x
fulminate|fulminat counterion ionable O,4@x,[N+]#[C-],x
thiocyanate|thiocyanat|sulfocyanate|sulfocyanat|sulfocyanide|sulfocyanid|rhodani
de|rhodanid counterion ionable S,4@x,C#N,x
isothiocyanate|isothiocyanat|isorhodanide|isorhodanid counterion ionable
N,4@x,=C=S,x
selenocyanate|selenocyanat counterion ionable [Se],4@x,C#N,x
isoselenocyanate|isoselenocyanat counterion ionable N,4@x,=C=[Se],x
tellurocyanate|tellurocyanat counterion ionable [Te],4@x,C#N,x
isotellurocyanate|isotellurocyanat counterion ionable N,4@x,=C=[Te],x
azide|azid counterion ionable N,4@x,=[N+]=[N-],x
sulfenamide|sulfenamid counterion counterion S,4@x,N,n
sulfonazide counterion counterion S,4@x,(=O)(=O)N[N+][N-],x
alcohol|icalcohol counterion counterion O,4@x
deuterol counterion counterion O,4@x,[2H],x
selenol counterion counterion [Se],4@s
tellurol counterion counterion [Te],4@s
nitrile|nitril counterion counterion N,12@x
carbonitrile|carbonitril counterion counterion C#N,4@x
diazonium counterion counterion [N+],4@x,#N,x
mercaptan|thioalcohol counterion counterion S,4@x
hydroperoxide|hydroperoxid counterion ionable O,4@x,O,x

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carboxaldehyde|carboxaldehyd|carboxyaldehyde|carboxyaldehyd|carbonal counterion
counterion C,4@x,(=O),x
carboxaldoxime|carboxaldoxim counterion counterion C,4@x,(=NO),x
carbamidine counterion counterion C,4@x,(=,x,N,1@n'|n2,),x,N,2@n|n1
oxyfluoride counterion bridge F,4@x,.,x,O,8@x
oxychloride counterion bridge Cl,4@x,.,x,O,8@x
oxybromide counterion bridge Br,4@x,.,x,O,8@x
oxyiodide counterion bridge I,4@x,.,x,O,8@x
thiochloride counterion bridge Cl,4@x,.,x,S,8@x
oxylradical counterion counterion O,20@x
carbo|carb carbeth root C,4@x,(=O),x
dioxyl infix infix O,4@x,O,x
oxy infix doublebondable O,4@x
peroxy infix doublebondable O,4@x,O,x
sulfanyl infix infix S,4@x
thio infix doublebondable S,4@x
mercapto infix infix S,4@x
seleno infix doublebondable [Se],4@x
telluro infix doublebondable [Te],4@x
amino|amin infix infix N,4@n|w|omega
phosphino infix infix P,4@n|w|omega
phosphinyl infix infix [PH3],4@x,(=,x,O,x,),x
arsino infix infix [As],4@n|w|omega
stibino infix infix [Sb],4@n|w|omega
bismuthino infix infix [Bi],4@n|w|omega
hydrazino infix infix N,2|n',N,4@1|n
hydroximino infix infix N,8@n,O,x
imino|imin infix infix N,8@n
imino|imin imine infix N,4@n
iminio infix infix [N+],8@n
iminio imine infix [N+],4@n
nitrilo infix infix N,12@n
hydrazono infix infix N,8@x,N,n
oximino infix infix N,8@x,O,o
amidosulfen infix infix S,x,N,n
sulfen infix infix S,x
sulfin infix doublebondable S,x,(=O),x
selenen infix infix [Se],x
carbonyl infix carbonyl C,4@x,(=O),x
thiocarbonyl infix carbonyl C,4@x,(=S),x
selenocarbonyl infix carbonyl C,4@x,(=[Se]),x
tellurocarbonyl infix carbonyl C,4@x,(=[Te]),x
thionyl infix carbonyl S,4@x,(=O),x
sulfuryl infix carbonyl S,4@x,(=O)(=O),x
carbonothioyl infix carbonyl C,4@x,(=S),x
carbonimidoyl infix carbonyl C,4@x,(=N),x
carbamo|carbam infix trivial C,x,(=,x,O,x,),x,N,n|w|omega
nitrilomethylidyne root bridge C,4@x,=,x,N,4@x
diazo azo diazo N,4@x,=,x,N,x
azo infix doublebondable N,4@x,=,x,N,x
azo root bridge N,4@x,=,x,N,4@x
azo azo root N,x,=,x,N,x
hydrazo infix doublebondable N,x,N,4@x
hydrazo root bridge N,4@x,N,4@x
hydrazo azo root N,1@x,N,1@x
nnoazoxy|azoxy infix doublebondable [N+],4@x,([O-]),x,=,x,N,x
nnoazoxy|azoxy root bridge [N+],4@x,([O-]),x,=,x,N,4@x
```

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azoxy azo root [N+],x,([O-]),x,=,x,N,x
azodioxy azo root [N+],x,([O-]),x,=,x,[N+],x,[O-],x
azodioxy infix doublebondable [N+],4@x,([O-]),x,=,x,[N+],x,[O-],x
azodioxy root bridge [N+],4@x,([O-]),x,=,x,[N+],4@x,[O-],x
onnazoxy|nonazoxy infix doublebondable N,4@x,=,x,[N+],x,[O-],x
diazoamino azo root N,x,=,x,N,x,N,n
diazoamino root bridge N,4@x,=,x,N,x,N,4@n
mercuri infix infix [Hg],4@x
per prefix permult x,x
bi prefix ringmult 2,mult
ter prefix ringmult 3,mult
quater prefix ringmult 4,mult
quinque prefix ringmult 5,mult
sexi prefix ringmult 6,mult
septi prefix ringmult 7,mult
octi prefix ringmult 8,mult
novi prefix ringmult 9,mult
deci prefix ringmult 10,mult
kis prefix kis 1,x
mono|mon prefix prefix 1,mult
hen prefix chainable 1,mult
di prefix prefix 2,mult
do prefix chainable 2,mult
bis prefix kis 2,mult
tri prefix chainable 3,mult
tris prefix kis 3,mult
tetr|tetra prefix chainable 4,mult
pent|penta prefix chainable 5,mult
hex|hexa prefix chainable 6,mult
hept|hepta prefix chainable 7,mult
oct|octa prefix chainable 8,mult
non|nona prefix chainable 9,mult
dec|deca prefix chainable 10,mult
undec|undeca prefix prefix 11,mult
eicos|eicosa|icos|icosa|cos|cosa prefix chainable 20,mult
uneicos|uneicosa|unicos|unicosa prefix prefix 21,mult
triacont|triaconta|tricont|triconta prefix chainable 30,mult
tetracont|tetraconta prefix chainable 40,mult
pentacont|pentaconta prefix chainable 50,mult
hexacont|hexaconta prefix chainable 60,mult
heptacont|heptaconta prefix chainable 70,mult
octacont|octaconta prefix chainable 80,mult
nonacont|nonaconta prefix chainable 90,mult
hect|hecta prefix chainable 100,mult
dict|dicta prefix chainable 200,mult
trict|tricta prefix chainable 300,mult
tetract|tetract prefix chainable 400,mult
pentact|pentacta prefix chainable 500,mult
hexact|hexact prefix chainable 600,mult
heptact|heptacta prefix chainable 700,mult
octact|octacta prefix chainable 800,mult
nonact|nonacta prefix chainable 900,mult
kili|kilia prefix chainable 1000,mult
dili|dilia prefix chainable 2000,mult
trili|trilia prefix chainable 3000,mult
tetrali|tetralia prefix chainable 4000,mult
pentali|pentalia prefix chainable 5000,mult
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hexali|hexalia prefix chainable 6000,mult
heptali|heptalia prefix chainable 7000,mult
octali|octalia prefix chainable 8000,mult
nonali|nonalia prefix chainable 9000,mult
cyclo cyclo cyclo 1,cyclo
spiro spiro unknown 1,spiro

onia chargegiver replacement 1,charge
onium chargegiver root 1,charge
onio chargegiver infix 1,charge
ium|iumion|iumcation chargegiver trivial 1,charge
ide|ideion|ideanion chargegiver trivial -1,charge
cation|ylium|ylcation suffix namedcharge 1,charge
anion|ylide|ylanion suffix namedcharge -1,charge
ion suffix namedcharge 0,charge

oxammonium root root O,x,[N+],x
ammonium|aminium root root [N+],n|omega
ammonio infix infix [N+],4@n
phosphonium root root [P+],x|omega
phosphonio infix infix [P+],4@x
arsonium root root [As+],x|omega
arsonio infix infix [As+],4@x
stibonium root root [Sb+],x|omega
stibonio infix infix [Sb+],4@x
bismuthonium root root [Bi+],x|omega
bismuthonio infix infix [Bi+],4@x
sulfonium root root [S+],s|omega
selenonium root root [Se+],s|omega
telluronium root root [Te+],s|omega
sulfoxonium root root [S+],s,=O,x
sulfonio infix infix [S+],4@s
chloronium root root [Cl+],x|omega
chloronio infix infix [Cl+],4@x
bromonium root root [Br+],x|omega
bromonio infix infix [Br+],4@x
iodonium root root [I+],x|omega
iodonio infix infix [I+],4@x

actina replacement replacement [Ac],x
alumina|alumin replacement replacement [Al],x
argenta|argent replacement replacement [Ag],x
arsa|ars|arsen replacement replacement [As],x
arsora|arsor replacement replacement [AsH5],x
astata|astat replacement replacement [At],x
aura replacement replacement [Au],x
aza|az replacement replacement N,n
bara replacement replacement [Ba],x
berkela|berkel replacement replacement [Bk],x
berylla|beryll replacement replacement [Be],x
bisma|bism replacement replacement [Bi],x
bora|bor replacement replacement [B],x
broma replacement replacement [Br],x
cadma|cadm replacement replacement [Cd],x
calca|calc replacement replacement [Ca],x
californa|californ replacement replacement [Cf],x
carba|carb replacement replacement [C],x
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cera|cer replacement replacement [Ce],x
chlora replacement replacement [Cl],x
chroma|chrom replacement replacement [Cr],x
cobalta replacement replacement [Co],x
cupra|cupr replacement replacement [Cu],x
cura replacement replacement [Cm],x
dysprosa|dyspros replacement replacement [Dy],x
einsteina|einstein replacement replacement [Es],x
europa|europ replacement replacement [Eu],x
ferma|ferm replacement replacement [Fm],x
ferra|ferr replacement replacement [Fe],x
fluora replacement replacement [F],x
gadolina|gadol replacement replacement [Gd],x
galla replacement replacement [Ga],x
germa|germ|german replacement replacement [Ge],x
hafna|hafn replacement replacement [Hf],x
holma|holm replacement replacement [Ho],x
inda replacement replacement [In],x
ioda replacement replacement [I],x
irida|irid replacement replacement [Ir],x
lanthana|lanthan replacement replacement [La],x
lawrenca|lawrenc replacement replacement [Lr],x
luteta|lutet replacement replacement [Lu],x
magnesa|magnes replacement replacement [Mg],x
mangana|mangan replacement replacement [Mn],x
mendeleva|mendelev replacement replacement [Md],x
mercura|mercur replacement replacement [Hg],x
molybda|molybd replacement replacement [Mo],x
neodyma|neodym replacement replacement [Nd],x
neptuna|neptun replacement replacement [Np],x
nickela replacement replacement [Ni],x
nioba|niob replacement replacement [Nb],x
nobela|nobel replacement replacement [No],x
osma|osm replacement replacement [Os],x
oxa|ox replacement replacement O,x
pallada|pallad replacement replacement [Pd],x
phospha|phosph replacement replacement P,x
phosphora|phosphor replacement phosphor [PH5],x
platina|platin replacement replacement [Pt],x
plumba|plumb replacement replacement [Pb],x
plutona|pluton replacement replacement [Pu],x
polona|polon replacement replacement [Po],x
praseodyma|praseodym replacement replacement [Pr],x
prometha|prometh replacement replacement [Pm],x
protactina|protactin replacement replacement [Pa],x
rada replacement replacement [Ra],x
rhena|rhen replacement replacement [Re],x
rhoda replacement replacement [Rh],x
ruthena|ruthen replacement replacement [Ru],x
samara|samar replacement replacement [Sm],x
scanda|scand replacement replacement [Sc],x
selena|selen replacement replacement [Se],x
sila|sil|silic replacement replacement [Si],x
stanna|stann replacement replacement [Sn],x
stiba|stib|antimon replacement replacement [Sb],x
stibora|stibor replacement replacement [SbH5],x
stronta|stront replacement replacement [Sr],x
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tantala|tantal replacement replacement [Ta],x
techneta|technet replacement replacement [Tc],x
tellura|tellur replacement replacement [Te],x
terba|terb replacement replacement [Tb],x
thalla|thall replacement replacement [Tl],x
thia|thi replacement replacement S,x
thora|thor replacement replacement [Th],x
thula|thul replacement replacement [Th],x
titana|titan replacement replacement [Ti],x
tungsta|tungst|wolframa|wolfram replacement replacement [W],x
urana|uran replacement replacement [U],x
vanada|vanad replacement replacement [V],x
ytterba|ytterb replacement replacement [Yb],x
yttra|yttr replacement replacement [Y],x
zinca replacement replacement [Zn],x
zircona|zircon replacement replacement [Zr],x

zirconyl|zirconyliv root setvalence [Zr++],x,(=O),x
vanadyliv|vanadyl root setvalence [V++],x,(=O),x
chromyl root setvalence [Cr++],x,(=O)(=O),x
uranyl root setvalence [U++],x,(=O)(=O),x

seleno|selen thio unknown [Se],x
telluro|tellur thio unknown [Te],x
thio|thi thio unknown S,x
i|iso tert iso 3,tert
sec tert sec 3,tert
s tert sec 4,tert
neo tert neo 4,tert
t|tert|tertiary tert tert 4,tert
imide|imid imide root N,n
imido|imidyl imide root N,4@n
chlorimide|chlorimid imide root NCl,x
imide root oxime N,8@n
chlorimide|chlorimid root oxime NCl,8@x
hexafluorophosphoricacid root root [H+].[P-](F)(F)(F)(F)(F)F,x
hexafluorosilicicacid root root [H+].[H+].[Si--](F)(F)(F)(F)(F)F,x
tetrafluoroboricacid root root [H+].[B-](F)(F)(F)F,x
hexafluorozirconicicacid root root [H+].[H+].[Zr--](F)(F)(F)(F)(F)F,x
nitramin cyanic cyanic N,1@x,[N+](=O)[O-],x
isocyan cyanic cyanic N,1@x,=C=O,x
isothiocyan cyanic cyanic N,1@x,=C=S,x
isoselenocyan cyanic cyanic N,1@x,=C=[Se],x
cyan cyanic cyanic O,1@x,C#N,x
hydrocyan cyanic cyanic [H]C#N,x
fulmin cyanic cyanic O,1@x,[N+]#[C-],x
hydrofluor cyanic cyanic [H]F,x
hydrochlor cyanic cyanic [H]Cl,x
hydrobrom cyanic cyanic [H]Br,x
hydroiod|hydriod cyanic cyanic [H]I,x
tetron cyanic cyanic O,1,Ring,Ring1,C,2,(=O),x,C,3,C,4,(=O),x,C,5,Ring,Ring1
osm cyanic cyanic [Os](=O)(=O)(=O)=O,x
xanth|xanthogen cyanic cyanic O,x,C,x,(=,x,S,x,),x,S,s|w|omega
rhodanin cyanic cyanic
S,1,Ring,Ring1,C,2,(=,x,S,x,),x,N,3,C,4,(=,x,O,x,),x,C,5,Ring,Ring1
ellag cyanic cyanic O=C3Oc1c(O)c(O)cc4c1c2c(OC4=O)c(O)c(O)cc23,x
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ur cyanic cyanic
N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,Ring,Ring2,N,9,C,8,(=O),x,N,7,C,5,=,x,Ring,Rin
g2,C,6,(=O),x,Ring,Ring1
squar|quadrat cyanic cyanic
O,1@x,C,x,Ring,Ring1,=,x,C,x,(,x,O,1@x,),x,C,x,(=O),x,C,x,(=O),x,Ring,Ring1
crocon cyanic cyanic
O,1@x,C,x,Ring,Ring1,=,x,C,x,(,x,O,1@x,),x,C,x,(=O),x,C,x,(=O),x,C,x,(=O),x,Ring
,Ring1
dehydroacet cyanic cyanic CC(C(C1=O)C(C=C(C)O1)=O)=O,x
ascorb|lascorb|ascorbyl|lascorbyl|isoascorb pseudosugar unknown x,x
ascorb|lascorb cyanic cyanic
O,x,C,3,Ring,Ring1,[C@@H],4,(,x,[C@@H],5,(,x,O,x,),x,C,6,O,x,),x,O,x,C,1,(=O),x,
C,2,(,x,O,x,),x,=,x,Ring,Ring1
ascorbyl|lascorbyl root root
O,x,C,3,Ring,Ring1,[C@@H],4,(,x,[C@@H],5,(,x,O,x,),x,C,6,O,x,),x,O,x,C,1,(=O),x,
C,2,(,x,O,x,),x,=,x,Ring,Ring1
isoascorb cyanic cyanic
O,x,C,3,Ring,Ring1,[C@@H],4,(,x,[C@H],5,(,x,O,x,),x,C,6,O,x,),x,O,x,C,1,(=O),x,C
,2,(,x,O,x,),x,=,x,Ring,Ring1
koj cyanic cyanic
o,1,Ring,Ring1,c,2,c,3,(O),x,c,4,(=O),x,c,5,c,6,(CO),x,Ring,Ring1
picrolon cyanic cyanic O=C1N(C2=CC=C([N+]([O-])=O)C=C2)N=C(C)C1[N+]([O-])=O,x
barbitur cyanic cyanic
N,1@1,Ring,Ring1,C,2,(=,x,O,x,),x,N,1@3,C,4,(=,x,O,x,),x,C,5,C,6,(=,x,O,x,),x,Ri
ng,Ring1
violur cyanic cyanic
N,1@1,Ring,Ring1,C,2,(=,x,O,x,),x,N,1@3,C,4,(=,x,O,x,),x,C,5,(=NO),x,C,6,(=,x,O,
x,),x,Ring,Ring1
isobarbitur cyanic cyanic
n,1,Ring,Ring1,c,2,(,x,O,1@x,),x,n,3,c,4,c,5,(,x,O,1@x,),x,c,6,(,x,O,1@x,),x,Rin
g,Ring1
cyanur cyanic cyanic
n,1,Ring,Ring1,c,2,(,x,O,1@x,),x,n,3,c,4,(,x,O,1@x,),x,n,5,c,6,(,x,O,1@x,),x,Rin
g,Ring1
isocyanur cyanic cyanic
N,1@1,Ring,Ring1,C,2,(=,x,O,x,),x,N,1@3,C,4,(=,x,O,x,),x,N,1@5,C,6,(=,x,O,x,),x,
Ring,Ring1
melanur cyanic cyanic
n,1,Ring,Ring1,c,2,(,x,O,1@x,),x,n,3,c,4,(,x,O,1@x,),x,n,5,c,6,(,x,N,1@x,),x,Rin
g,Ring1
rhodizon cyanic cyanic
C,1,Ring,Ring1,(,x,O,1@x,),x,=,x,C,2,(,x,O,1@x,),x,C,3,(=O),x,C,4,(=O),x,C,5,(=O
),x,C,6,(=O),x,Ring,Ring1
chloranil cyanic cyanic
c,1,Ring,Ring1,(=O),x,c,2,(Cl),x,c,3,(,x,O,1@x,),x,c,4,(=O),x,c,5,(Cl),x,c,6,(,x
,O,1@x,),x,Ring,Ring1
bromanil cyanic cyanic
c,1,Ring,Ring1,(=O),x,c,2,(Br),x,c,3,(,x,O,1@x,),x,c,4,(=O),x,c,5,(Br),x,c,6,(,x
,O,1@x,),x,Ring,Ring1
bromanil root root
c,1,Ring,Ring1,(=O),x,c,2,(Br),x,c,3,(Br),x,c,4,(=O),x,c,5,(Br),x,c,6,(Br),x,Rin
g,Ring1
nitranil cyanic cyanic c,1,Ring,Ring1,(=O),x,c,2,([N+]([O-
])=O),x,c,3,(,x,O,1@x,),x,c,4,(=O),x,c,5,([N+]([O-
])=O),x,c,6,(,x,O,1@x,),x,Ring,Ring1
picr cyanic cyanic O,1@x,c,1,Ring,Ring1,c,2,([N+]([O-])=O),x,c,3,c,4,([N+]([O-
])=O),x,c,5,c,6,([N+]([O-])=O),x,Ring,Ring1

picryl root root c,4@1,Ring,Ring1,c,2,([N+]([O-])=O),x,c,3,c,4,([N+]([O-
])=O),x,c,5,c,6,([N+]([O-])=O),x,Ring,Ring1
styphn cyanic cyanic O,1@x,c,1,Ring,Ring1,c,2,([N+]([O-
])=O),x,c,3,(,x,O,1@x,),x,c,4,([N+]([O-])=O),x,c,5,c,6,([N+]([O-
])=O),x,Ring,Ring1
pyrophosphor cyanic cyanic
P,x,(=O),x,(,x,O,1@x,),x,(,x,O,1@x,),x,O,x,P,x,(=O),x,(,x,O,1@x,),x,O,1@x
dithiopyrophosphor cyanic cyanic
P,x,(=S),x,(,x,O,1@x,),x,(,x,O,1@x,),x,O,x,P,x,(=S),x,(,x,O,1@x,),x,O,1@x
peroxydisulf cyanic cyanic
S,x,(=O)(=O),x,(,x,O,1@x,),x,OO,x,S,x,(=O)(=O),x,O,1@x
pyrosulf cyanic cyanic S,x,(=O)(=O),x,(,x,O,1@x,),x,O,x,S,x,(=O)(=O),x,O,1@x
isethion cyanic cyanic O,1@x,S,x,(=O)(=O),x,C,1,C,2,O,o
hydrosulfite|dithionite root root S,x,(=O),x,(,x,[O-],x,),x,S,x,(=O),x,[O-],x
dithionate root root S,x,(=O)(=O),x,(,x,[O-],x,),x,S,x,(=O)(=O),x,[O-],x
cacodyl cyanic cyanic [As](=O)(,x,O,1@x,)(C)C,x
chromotrop cyanic cyanic
c,4,Ring,Ring1,c,3,(S(=O)(=O),x,O,1@x,),x,c,2,c,1,(O),x,c,8a,Ring,Ring2,c,8,(O),
x,c,7,c,6,(S(=O)(=O),x,O,1@x,),x,c,5,c,4a,Ring,Ring1,Ring,Ring2
acid endercyanic unknown x,x
ochloranil root root
c,1,Ring,Ring1,(=O),x,c,2,(=O),x,c,3,(Cl),x,c,4,(Cl),x,c,5,(Cl),x,c,6,(Cl),x,Rin
g,Ring1
mchloranil root root
c,1,Ring,Ring1,(=O),x,c,2,(Cl),x,c,3,(=O),x,c,4,(Cl),x,c,5,(Cl),x,c,6,(Cl),x,Rin
g,Ring1
pchloranil|spergon root root
c,1,Ring,Ring1,(=O),x,c,2,(Cl),x,c,3,(Cl),x,c,4,(=O),x,c,5,(Cl),x,c,6,(Cl),x,Rin
g,Ring1
ate organometallicanion ate x,x
icacid|oicacid acid acid O,8@x,.,,x,O,5@x
ate|oate acid ate O,8@x,.,,x,O,5@x
ic|oic acid ic O,8@x,.,,x,O,5@x
ous acid ous O,5@x
ite acid ite O,5@x
amido acid infix O,8@x,.,,x,N,5@n
amido part2acid infix N,5@n
acid part2acid acid O,5@x
amide|amid part2acid amide N,6@n
amide|amid acid acid O,8@x,.,,x,N,6@n
chloramide|chloramid part2acid amide N,5@n,Cl,x
bromamide|bromamid part2acid amide N,5@n,Br,x
amidine|amidin|imidamide acid acid N,9@n'|n2,.,,x,N,6@n|n1
amidrazone|amidrazon acid acid N,9@n'',.,,x,N,5@n|n1,N,2@n'|n2
hydrazide|hydrazid|ohydrazide|ohydrazid acid acid
O,8@x,.,,x,N,5@n|1|n1,N,2@n'|2|n2
hydrazide|hydrazid part2acid amide N,5@n|1|n1,N,2@n'|2|n2
onitrile|nitrile acid nitrile N,12@x
nitrile|anammonide part2acid nitrile N,12@x
ether part2acid acid O,4@x,C,x,C,x
oyl acid makefree O,8@x
basic basic unknown [H],4@x
aldehyde|aldehyd part2acid acid H,4@x
aldehyde|aldehyd|al acid acid O,8@x,.,,x,H,4@x
aldoxime|aldoxim acid acid H,4@x,.,,x,N,8@x,O,o
aldimine|aldimin acid acid H,4@x,.,,x,N,8@n
lacton|lactone part2acid lactone O,5@x

thiolacton|thiolactone part2acid lactone S,5@x
selenolacton|selenolactone part2acid lactone [Se],5@x
tellurolacton|tellurolactone part2acid lactone [Te],5@x
lacton|lactone|olacton|olactone|iclacton|iclactone|olide|olid acid lactone
O,8@x,.,x,O,5@x
lactam part2acid lactone N,5@x
lactam|olactam|iclactam acid lactone O,8@x,.,x,N,5@x
lactim part2acid lactone N,9@x
lactim|olactim|iclactim acid lactone O,4@x,.,x,N,9@x
sulfimide part2acid lactone N,4@x,S,1@x,(=O)(=O),x
anilide|analide acid acid
O,8@x,.,x,N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),
x
anilide|analide part2acid amide
N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),x
anilido|analido acid infix
O,8@x,.,x,N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),
x
anilido|analido part2acid infix
N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),x
4nitroanilide|pnitroanilide acid acid
O,8@x,.,x,N,4@n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=O)[O-
]),x,c,5',c,6',Ring,Ring1,),x
4nitroanilide|pnitroanilide part2acid acid
N,4@n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=O)[O-
]),x,c,5',c,6',Ring,Ring1,),x
morpholide acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
morpholide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
ophenone acid acid
O,8@x,.,x,c,4@1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
ophenone part2acid acid
c,4@1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
onaphthone acid acid
O,8@x,.,x,c,4@1',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',
c,8a',Ring,Ring1,Ring,Ring2
onaphthone part2acid acid
c,4@1',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',c,8a',Ring
,Ring1,Ring,Ring2
ureide acid acid O,8@x,.,x,N,4@n,C(=O),x,N,n'
ureide part2acid amide N,4@n,C(=O),x,N,n'
piperazide acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
piperazide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
piperidide acid acid O,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,C,x,Ring,Ring1
piperidide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,C,x,Ring,Ring1
anhydride|cyclicanhydride part2acid anhydride O,5@x
thioanhydride part2acid anhydride S,5@x
selenoanhydride part2acid anhydride [Se],5@x
telluroanhydride part2acid anhydride [Te],5@x
imid|imide part2acid anhydride N,5@x
cyclam root root S,x,(=O)(=O),x,(NC1CCCCC1),x,O,1@x
atrop loveracid root
C,x,C,x,(,x,=,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6
,Ring,Ring1
pinon loveracid root CCC1CC(C(C)(C)1)C(=O)C,x
benzil loveracid root
C,x,C,a|alpha,(,x,O,x,),x,(,x,c,1,Ring,Ring1,=,x,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,
),x,c,1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2

glycoll|glycol loveracid alkane C,x,C,2|w|omega,O,x
thioglycoll|thioglycol loveracid root C,x,C,2,S,w|omega
selenoglycoll|selenoglycol loveracid root C,x,C,2,[Se],w|omega
telluroglycoll|telluroglycol loveracid root C,x,C,2,[Te],w|omega
boro|bor|orthobor loveracid root [B],x,(,x,O,1@o'',),x,(,x,O,1@o',),x,O,1@o
metabor loveracid root [B],x,(,x,=,x,O,o',),x,O,1@o
perbor loveracid root [B],x,(,x,=,x,O,x,)(,x,=,x,O,x,),x,O,1@o
borin loveracid root [B],x,O,1@o
borono|boron loveracid counterion [B],4@x,(,x,O,1@o',),x,O,1@o
diphosphor|pyrophosphor|pyrophosph loveracid root
P,a|alpha,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,O,x,)(,x,O,
1@o'''|p2,),x,O,1@o''''
dithiodiphosphor|dithiopyrophosphor|dithiopyrophosph loveracid root
P,a|alpha,(=,x,S,x,)(,x,O,1@o'',)(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,S,x,)(,x,O,
1@o'''|p2,),x,O,1@o''''
phosphosulf loveracid root
P,a|alpha,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,O,x,S,b|beta,(=,x,O,x,)(=,x,O,x,
),x,O,1@o'''
glycerophosph|alphaglycerophosph|lalphaglycerophosph|dalphaglycerophosph|dlalpha
glycerophosph loveracid root
P,a|alpha,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,OCC(O)CO,x
glycerophospho|alphaglycerophospho|lalphaglycerophospho|dalphaglycerophospho|dla
lphaglycerophospho loveracid root
P,4@a|alpha,(=,x,O,x,)(,x,O,1@o',),x,OCC(O)CO,x
triphosphor loveracid root
P,a|alpha,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,O,x,)(,x,O,
1@o'''|p2,),x,O,x,P,g|gamma,(=,x,O,x,)(,x,O,1@o'''',),x,O,1@o'''''|p3
2thiodiphosphor loveracid root
P,a|alpha,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,S,x,)(,x,O,
1@o'''|p2,),x,O,1@o''''
3thiotriphosphor loveracid root
P,a|alpha,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,O,x,)(,x,O,
1@o'''|p2,),x,O,x,P,g|gamma,(=,x,S,x,)(,x,O,1@o'''',),x,O,1@o'''''|p3
tetraphosphor loveracid root
P,a|alpha,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,O,x,)(,x,O,
1@o'''|p2,),x,O,x,P,g|gamma,(=,x,O,x,)(,x,O,1@o'''',),x,O,o'''''|p3,P,d|delta,(=
,x,O,x,)(,x,O,1@o''''''',),x,O,1@o'''''''|p4
phosphoro|phosphor|phosph|orthophosph|orthophosphor loveracid root
P,x,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,O,1@o
phosphono|phosphon loveracid counterion P,4@x,(=,x,O,x,)(,x,O,1@o',),x,O,1@o
phospheno|phosphen loveracid root P,x,(=,x,O,x,)(=,x,O,x,),x,O,1@o
hypophosph loveracid root [PH0],x,(=,x,O,x,)(=,x,O,x,),x,O,1@o
phosphino|phosphin loveracid root [PH2],x,(=,x,O,x,),x,O,1@o
phosphoenolpyruv loveracid root   .
P,x,(=,x,O,x,)(,x,O,1@o',)(,x,O,1@o,),x,O,x,C,x,(=C),x,C,x,(=O),x,O,1@x
phyt loveracid root
O=P(,x,O,1@x,)(,x,O,1@x,)O[C@H]1[C@@H](OP(,x,O,1@x,)(,x,O,1@x,)=O)[C@@H](OP(,x,O
,1@x,)(,x,O,1@x,)=O)[C@H](OP(,x,O,1@x,)(,x,O,1@x,)=O)[C@@H](OP(,x,O,1@x,)(,x,O,1
@x,)=O)[C@@H]1OP(,x,O,1@x,)(,x,O,1@x,)=O,x
orthoarsen|arseno|arsen loveracid root
[As],x,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,O,1@o
arsenicacid root root [As],x,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,O,1@o
arsono|arson loveracid counterion [As],4@x,(=,x,O,x,)(,x,O,1@o',),x,O,1@o
arsino|arsin loveracid root [AsH2],x,(=,x,O,x,),x,O,1@o
stibeno|stiben|antimon loveracid root
[Sb],x,(=,x,O,x,)(,x,O,1@o'',)(,x,O,1@o',),x,O,1@o
stibono|stibon loveracid counterion [Sb],4@x,(=,x,O,x,)(,x,O,1@o',),x,O,1@o

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nitr loveracid root [N+],x,(,x,O,1@x,)(=,x,O,x,),x,[O-],x
sulfono|sulfon loveracid counterion S,4@x,(=O),x,(=O),x,O,1@x
sulfino|sulfin loveracid counterion S,4@x,(=O),x,O,1@x
sulfeno|sulfen loveracid counterion S,4@x,O,1@x
selenono|selenon loveracid counterion [Se],4@x,(=O),x,(=O),x,O,1@x
selenino|selenin loveracid counterion [Se],4@x,(=O),x,O,1@x
tellurono|telluron loveracid counterion [Te],4@x,(=O),x,(=O),x,O,1@x
tellurino|tellurin loveracid counterion [Te],4@x,(=O),x,O,1@x
carbox|carboxyl|carbo|carb loveracid counterion C,4@x
carbon|carbono loveracid root C,x,O,1@o
bicarbon|bicarbono loveracid root C,x,O,o,[H],x
mangan loveracid root [Mn],x,(=O)(=O),x,(,x,O,o',),x,O,1@o
permangan loveracid root [Mn],x,(=O)(=O)(=O),x,O,1@o
perrhen loveracid root [Re],x,(=O)(=O)(=O),x,O,1@o
perruthen loveracid root [Ru],x,(=O)(=O)(=O),x,O,1@o
ruthen loveracid root [Ru],x,(=O)(=O)(=O),x,(,x,O,o',),x,O,1@o
niob loveracid root [Nb],x,(=O)(=O),x,O,1@o
zircon loveracid root [Zn],x,(=O),x,(,x,O,o',),x,O,1@o
tantal loveracid root [Ta],x,(=O)(=O),x,O,1@o
metaphosph|metaphosphor loveracid root P,x,(=O)(=O),x,O,1@o
bismuth loveracid root [Bi],x,(=O)(=O),x,O,1@o
alumin loveracid root [Al],x,(=O),x,O,1@o
dichrom|bichrom loveracid root
[Cr],x,(=O)(=O)(,x,O,1@o',),x,O,x,[Cr],x,(=O)(=O),x,O,1@o
chrom loveracid root [Cr],x,(=O)(=O)(,x,O,1@o',),x,O,1@o
tungst|wolfram loveracid root [W],x,(=O)(=O)(,x,O,1@o',),x,O,1@o
molybd loveracid root [Mo],x,(=O)(=O)(,x,O,1@o',),x,O,1@o
silic|metasilic loveracid root [Si],x,(=O)(,x,O,1@o',),x,O,1@o
stann loveracid root [Sn],x,(=O)(,x,O,o',),x,O,1@o
titan loveracid root [Ti],x,(=,x,O,x,)(,x,O,1@o',),x,O,1@o
trifl loveracid root
S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,C,x,(,x,F,x,)(,x,F,x,),x,F,x
naphthion loveracid root
S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,c1ccc(N)c2ccccc12,x
sulfur|sulf loveracid root S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,O,1@o
chlorosulfamicacid root root S,x,(=O)(=O)(Cl),1@x,N,w|omega
sulfam root root S,x,(=O),x,(=O),x,(O),1@x,N,w|omega
sulfamide|sulfamid root root S,x,(=O),x,(=O),x,(,x,N,1@n',),x,N,n
seleni|selen loveracid root [Se],x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,O,1@o
telluri|tellur loveracid root [Te],x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,O,1@o
sulfanil loveracid root
S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4
,(,x,N,n|n4,),x,c,5,c,6,Ring,Ring1
sulfanilamide root root
N,n|n1,S,x,(=,x,O,x,)(,x,=O,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n'|n4,),x,c,5
,c,6,Ring,Ring1
sulfanilamido root root
N,4@x,S,x,(=,x,O,x,)(,x,=O,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n|n4,),x,c,5,c
,6,Ring,Ring1
sulfanilyl root root
S,4@x,(=,x,O,x,)(,x,=O,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n,),x,c,5,c,6,Ring
,Ring1
orthanil loveracid root
S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,c,1,Ring,Ring1,c,2,(,x,N,n,),x,c,3,c,4,c,
5,c,6,Ring,Ring1
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metanil loveracid root
S,x,(=,x,O,x,)(,x,=O,x,)(,x,O,1@o',),x,c,1,Ring,Ring1,c,2,c,3,(,x,N,n,),x,c,4,c,
5,c,6,Ring,Ring1
metanilyl root root
S,4@x,(=,x,O,x,)(,x,=O,x,),x,c,1,Ring,Ring1,c,2,c,3,(,x,N,n,),x,c,4,c,5,c,6,Ring
,Ring1
vanad|metavanad loveracid root [V],x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
orthovanad loveracid root [V],x,(=,x,O,x,)(,x,O,o'',)(,x,O,o',),x,O,1@o
fluor loveracid root F,x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
chlor loveracid root Cl,x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
brom loveracid root Br,x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
iod loveracid root I,x,(=,x,O,x,)(,x,=O,x,),x,O,1@o
metaperiod loveracid root I,x,(=,x,O,x,)(=,x,O,x,)(,x,=O,x,),x,O,1@o
paraperiod loveracid root
I,x,(=,x,O,x,)(,x,O,1@o'''',)(,x,O,1@o''',)(,x,O,1@o'',)(,x,O,1@o',),x,O,1@o
semialdehyde tailderiverdiacid acid H,4@x
aldehyd deriverdiacid acid O,8@x,.,x,H,4@x
am deriverdiacid acid O,8@x,.,x,N,6@n
anil deriverdiacid acid
O,8@x,.,x,N,4@n,c,x,Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Ring1
bromo|brom deriveracid loveracidderiver Br,4@x
chloro|chlor deriveracid loveracidderiver Cl,4@x
fluoro|fluor deriveracid loveracidderiver F,4@x
cyano deriveracid loveracidderiver C,4@x,#N,x
iodo|iod deriveracid loveracidderiver I,4@x
amido|amid deriveracid loveracidderiver N,6@n
anilido deriveracid loveracidderiver
N,4@n,c,x,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
morpholino deriveracid loveracidderiver
N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
azido|azid deriveracid loveracidderiver N,4@x,=[N+]=[N-],x
bromido|bromid deriveracid acid Br,4@x
bromo|brom deriveracid loveracidderiver Br,4@x
chlorido|chlorid deriveracid acid Cl,4@x
choro|chlor deriveracid loveracidderiver Cl,4@x
cyanatido|cyanatid deriveracid acid O,4@x,C#N,x
cyanido|cyanid deriveracid acid C,4@x,#N,x
cyano deriveracid loveracidderiver C,4@x,#N,x
fluorido|fluorid deriveracid acid F,4@x
fluoro|fluor deriveracid loveracidderiver F,4@x
hydroxam|ohydroxam deriveracid acid N,5@n,O,x
hydroxim|ohydroxim deriveracid acid N,8@n,O,x
hydrazon|ohydrazon deriveracid acid N,8@x,N,n
iodido|iodid deriveracid acid I,4@x
iodo|iod deriveracid loveracidderiver I,4@x
isocyanatido|isocyanatid deriveracid acid N,4@x,=C=O,x
isocyanido|isocyanid deriveracid acid [N+],4@x,#[C-],x
thiocyanatido|thiocyanatid deriveracid acid S,4@x,C#N,x
isothiocyanatido|isothiocyanatid deriveracid acid N,4@x,=C=S,x
imido|imid deriveracid acid N,8@n
hydrazido|hydrazid deriveracid acid N,5@n|1',N,2@n'|2'
peroxo|perox|peroxy deriveracid acid O,4@x,O,1@oo
dithioperoxy deriveracid acid S,4@x,S,1@ss
seleno|selen deriveracid acid [Se],8@se
telluro|tellur deriveracid acid [Te],8@te
thio|thi|thion|thiono deriveracid acid S,8@s
thiolo|thiol deriveracid acid S,5@s
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per peracid peracid x,x
hypo peracid hypoacid x,x
etine|etin|etene|eten heterocyc oline C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
oline|olin|olene|olen heterocyc oline C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
isoxazoline|isoxazolin|isoazoline|isoazolin root oline
O,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
isothiazoline|isothiazolin root oline S,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
isoselenazoline|isoselenazolin root oline
[se],1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
pyrroline|pyrrolin root oline N,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
pyrazoline|pyrazolin root oline N,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
pyrazolino root oline N,4@1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
imidazoline|imidazolin root oline C,2,Ring,Ring1,N,3,C,4,C,5,N,1,Ring,Ring1
sulfolene|sulfolen root oline
S,1,(=,x,O,x,)(=,x,O,x,),x,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
sulfol root root
S,1,(=,x,O,x,)(=,x,O,x,),x,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
iridine|iridin heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,Ring,Ring1
etidin|etidine heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
olidine|olidin|olid heterocyc heterocyc
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
irene|irine|irin|iren heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,Ring,Ring1
ireno|irino|irin|iren opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,Ring,Ring1
irane|iran heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,Ring,Ring1
ete|et heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,Ring,Ring1
eto opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,Ring,Ring1
etane|etan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
ole|ol heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
olo opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
olane|olan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
ine|in heterocyc ine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
ino opfuser ine c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
inine|inin heterocyc inine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
ane|an heterocyc ane
C,1,Ring,Ring1,C,2|o|ortho,C,3|m|meta,C,4|p|para,C,5,C,6,Ring,Ring1
inane|inan heterocyc inan
C,1,Ring,Ring1,C,2|o|ortho,C,3|m|meta,C,4|p|para,C,5,C,6,Ring,Ring1
epane|epan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,Ring,Ring1
epine|epin heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,Ring,Ring1
epino opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,Ring,Ring1
ocane|ocan heterocyc heterocyc
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,Ring,Ring1
ocine|ocin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,Ring,Ring1
ocino opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,Ring,Ring1
onane|onan heterocyc heterocyc
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,Ring,Ring1
onine|onin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,Ring,Ring1
onino opfuser heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,Ring,Ring1
ecane|ecan heterocyc heterocyc
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,Ring,Ring1
ecine|ecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,Ring,Ring1
```

ecino|ecin opfuser heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,C,9,c,10,Ring,Ring1
cyclodecine|cycloundecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,Ring,Ring1
cycloundecine|cycloundecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,Ring,Ring1
cyclododecine|cyclododecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,Ring,Ring1
cyclotridecine|cyclotridecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,Ring,Ring1
cyclotetradecine|cyclotetradecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,Ring,Rin
g1
cyclopentadecine|cyclopentadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,Rin
g,Ring1
cyclohexadecine|cyclohexadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,Ring,Ring1
cycloheptadecine|cycloheptadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,c,17,Ring,Ring1
cyclooctadecine|cyclooctadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,c,17,c,18,Ring,Ring1
cyclononadecine|cyclononadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,c,17,c,18,c,19,Ring,Ring1
salt|salts|deriv|derivative salt unknown x,x
saltof salt saltof x,x
ester|esters ester unknown x,x
esterswith|estersof|esterwith|esterof ester esterwith x,x
ylene|ylen|ylenediyl ylene ylene x,x
0 roman unknown 0,x
i|1+|+1 roman unknown 1,x
ii|2+|+2 roman unknown 2,x
iii|3+|+3 roman unknown 3,x
iv|4+|+4 roman unknown 4,x
v|5+|+5 roman unknown 5,x
vi|6+|+6 roman unknown 6,x
vii|7+|+7 roman unknown 7,x
viii|8+|+8 roman unknown 8,x
ix|9+|+9 roman unknown 9,x
h hydroh unknown [H],4@x
hydro root hydroroot [H],4@x
annulene annulene unknown x,x
crown crown unknown x,x
cis+trans unknown unknown x,x
vitamin unknown unknown x,x
support unknown unknown x,x
deposition unknown unknown x,x
tion|ition unknown unknown x,x
electron unknown unknown x,x
pesticide unknown unknown x,x
16n|15n|14n nothandled nothandled x,x
99m nothandled nothandled x,x
nonoxynol nothandled nothandled x,x

```
kiton nothandled nothandled x,x
resinol nothandled nothandled x,x
mersol nothandled nothandled x,x
american nothandled nothandled x,x
turmeric nothandled nothandled x,x
phenacid|phenacide nothandled nothandled x,x
sulfurized nothandled nothandled x,x
branched nothandled nothandled x,x
carbor nothandled nothandled x,x
cuproxoline nothandled nothandled x,x
dioxygenyl nothandled nothandled x,x
cyclodextrin nothandled nothandled x,x
octapren|hexapren|undecapren nothandled nothandled x,x
oato|ato nothandled nothandled x,x
camphorato|camphorate nothandled nothandled x,x
acetonide nothandled nothandled x,x
alcoholate nothandled nothandled x,x
cyclobutoic nothandled nothandled x,x
fucoidan nothandled nothandled x,x
margarite nothandled nothandled x,x
pyrite nothandled nothandled x,x
glycerite nothandled nothandled x,x
pyroxylin nothandled nothandled x,x
cosmoline|cosmetol nothandled nothandled x,x
cupricol|cuproxol nothandled nothandled x,x
alol nothandled nothandled x,x
prenolone nothandled nothandled x,x
cergona nothandled nothandled x,x
platinol nothandled nothandled x,x
antin nothandled nothandled x,x
germanin nothandled nothandled x,x
phosphomolyb nothandled nothandled x,x
anhydro nothandled nothandled x,x
base nothandled nothandled x,x
thioflavin|thioflavine nothandled nothandled x,x
dionate|dionato nothandled nothandled x,x
doxyl nothandled nothandled x,x
acetylacetonato nothandled nothandled x,x
naphtholas nothandled nothandled x,x
compounded nothandled nothandled x,x
ketopinic nothandled nothandled x,x
indoxyl nothandled nothandled x,x
indo nothandled nothandled x,x
sulfobetaine nothandled nothandled x,x
coenzyme nothandled nothandled x,x
chlorin nothandled nothandled x,x
dehydro nothandled nothandled x,x
benzothiolate nothandled nothandled x,x
benzanthren nothandled nothandled x,x
mg nothandled nothandled x,x
vinglycin nothandled nothandled x,x
calanolide nothandled nothandled x,x
perbor nothandled nothandled x,x
dionato|dionate|acetonate nothandled nothandled x,x
tetraborate nothandled nothandled x,x
mefluidide nothandled nothandled x,x
decavanadate nothandled nothandled x,x
```

benzin nothandled nothandled x,x
dodecin nothandled nothandled x,x
methin nothandled nothandled x,x
- nothandled nothandled x,x
tolane nothandled nothandled x,x
monocrotaline nothandled nothandled x,x
adiphenine nothandled nothandled x,x
anhydridewith nothandled nothandled x,x
terpin nothandled nothandled x,x
thiuram nothandled nothandled x,x
acaprazine nothandled unknown x,x
acaralate nothandled unknown x,x
acetazide nothandled unknown x,x
acetazolamide root root CC(NC1=NN=C(S(N)(=O)=O)S1)=O,x
acetene nothandled unknown x,x
acetohexamide nothandled unknown x,x
acetonanyl nothandled unknown x,x
aconitine nothandled unknown x,x
alipamide nothandled unknown x,x
ambrosin nothandled unknown x,x
amygdalin nothandled unknown x,x
anisene nothandled unknown x,x
anisindione nothandled unknown x,x
antichlor nothandled unknown x,x
antiethanol nothandled unknown x,x
antiformin nothandled unknown x,x
antiphen nothandled unknown x,x
arsamin nothandled unknown x,x
arsenal nothandled unknown x,x
arsenolite nothandled unknown x,x
atolide nothandled unknown x,x
azamethone nothandled unknown x,x
azinthiamide nothandled unknown x,x
azobutyl nothandled unknown x,x
azolimine nothandled unknown x,x
azopyrin nothandled unknown x,x
benzilan nothandled unknown x,x
benzilen nothandled unknown x,x
benzolene nothandled unknown x,x
benzolin nothandled unknown x,x
benzone nothandled unknown x,x
benzoxonium nothandled unknown x,x
benztropine|benzotropine root root CN3C4CC(CC3CC4)OC(C2=CC=CC=C2)C1=CC=CC=C1,x
biamine nothandled unknown x,x
bichlorendo nothandled unknown x,x
biclofibrate nothandled unknown x,x
biformylchlorazin nothandled unknown x,x
biphenate nothandled unknown x,x
bisoxyphen nothandled unknown x,x
blauramine nothandled unknown x,x
borolin nothandled unknown x,x
boroxine nothandled unknown x,x
bromacrylide nothandled unknown x,x
bromamide nothandled unknown x,x
bromethalin nothandled unknown x,x
bromhexine root root CN(C2CCCCC2)CC1=C(N)C(Br)=CC(Br)=C1,x
brominal nothandled unknown x,x

bromobutide nothandled unknown x,x
bromol nothandled unknown x,x
bromopropylate nothandled unknown x,x
bromoxanide nothandled unknown x,x
brompyrazon nothandled unknown x,x
butalamine nothandled unknown x,x
butamid nothandled unknown x,x
butethamine nothandled unknown x,x
butethanol nothandled unknown x,x
butoctamide nothandled unknown x,x
butonate nothandled unknown x,x
butone nothandled unknown x,x
butoxylate nothandled unknown x,x
butylenin nothandled unknown x,x
butylpyrin nothandled unknown x,x
calcion root root [O-]S(=O)(C1=CC(C=C(S([O-])(=O)=O)C(N=NC4=CC(S([O-
])(=O)=O)=CC5=C4C=C(O)C=C5S([O-])(=O)=O)=C3O)=C3C(N=NC2=C(S([O-
])(=O)=O)C=C6C(C(O)=CC(S([O-
])(=O)=O)=C6)=C2O)=C1)=O.[Na+].[Na+].[Na+].[Na+].[Na+].[Na+],x
camphorene nothandled unknown x,x
carbamine nothandled unknown x,x
carbamite nothandled unknown x,x
carbromal nothandled unknown x,x
carbutamide nothandled unknown x,x
carbylamine nothandled unknown x,x
cardiamid nothandled unknown x,x
cardiamine nothandled unknown x,x
cardiol nothandled unknown x,x
caryne nothandled unknown x,x
cetamid nothandled unknown x,x
chelidonine root root CN5CC1=C(C6C(CC4=CC3=C(C=C4C56)OCO3)O)C=CC2=C1OCO2,x
chinacrin|chinacrine nothandled unknown x,x
chinoform nothandled unknown x,x
chinoleine nothandled unknown x,x
chloralose nothandled unknown x,x
chlorazine nothandled unknown x,x
chlorbicyclen nothandled unknown x,x
chlorbisan nothandled unknown x,x
chlorbutol nothandled unknown x,x
chlorethate nothandled unknown x,x
chlorindan nothandled unknown x,x
chlorisopropamide nothandled unknown x,x
chlormethine nothandled unknown x,x
chloroazodian nothandled unknown x,x
chlorobutin nothandled unknown x,x
chloroepoxide nothandled unknown x,x
chloronaphthine nothandled unknown x,x
chloropropamide nothandled unknown x,x
chloropropylate nothandled unknown x,x
chloropyramine root root ClC1=CC=C(C=C1)CN(C2=CC=CC=N2)CCN(C)C,x
chlorothen nothandled unknown x,x
chlorothenylpyramine nothandled unknown x,x
chlorotrisin nothandled unknown x,x
chloroxylenol nothandled unknown x,x
chlorphenamine nothandled unknown x,x
chlortalidone nothandled unknown x,x
chlorthiamid nothandled unknown x,x

```
chlorthioamide nothandled unknown x,x
cinchonamine nothandled unknown x,x
cineol|cineole nothandled unknown x,x
citralite nothandled unknown x,x
citrene nothandled unknown x,x
citronyl nothandled unknown x,x
citrylone nothandled unknown x,x
coniferin nothandled unknown x,x
cresotine nothandled unknown x,x
crotepoxide nothandled unknown x,x
crotonylene nothandled unknown x,x
cupricin nothandled unknown x,x
cyanogenamide nothandled unknown x,x
cyclamen nothandled unknown x,x
cyclobutyrol nothandled unknown x,x
cyclopentamine nothandled unknown x,x
cyclopentolate root root CN(CCOC(C(C2(CCCC2)O)C1=CC=CC=C1)=O)C,x
daconit nothandled unknown x,x
dazidamine nothandled unknown x,x
decitropine nothandled unknown x,x
delphinine nothandled unknown x,x
diazan nothandled unknown x,x
diazepan nothandled unknown x,x
dibrompropamidine nothandled unknown x,x
dibutin nothandled unknown x,x
dichlordiphenprop nothandled unknown x,x
dimethacrin nothandled unknown x,x
dimethoxanate nothandled unknown x,x
dimidazon nothandled unknown x,x
diodoxylin nothandled unknown x,x
dioxybenzone root root O=C(C2=CC=C(OC)C=C2O)C1=C(O)C=CC=C1,x
diphenoxylate root root
CCOC(C1(C4=CC=CC=C4)CCN(CCC(C2=CC=CC=C2)(C3=CC=CC=C3)C#N)CC1)=O,x
diphenylpyraline root root CN1CCC(OC(C3=CC=CC=C3)C2=CC=CC=C2)CC1,x
disilyn nothandled unknown x,x
disobutamide nothandled unknown x,x
dithiazanine nothandled unknown x,x
dothiepin nothandled unknown x,x
doxaminol nothandled unknown x,x
doxaprost nothandled unknown x,x
doxepin root root CN(C)CCC=C1C3=C(C=CC=C3)OCC2=C1C=CC=C2,x
doxopin nothandled unknown x,x
efuranol nothandled unknown x,x
endocet nothandled unknown x,x
endoiodin nothandled unknown x,x
esorb nothandled unknown x,x
estilben nothandled unknown x,x
ethamide nothandled unknown x,x
ethide nothandled unknown x,x
ethinamide nothandled unknown x,x
ethine nothandled unknown x,x
ethionamide root root NC(C1=CC(CC)=NC=C1)=S,x
ethoxazene nothandled unknown x,x
ethylan nothandled unknown x,x
ethylhexaldehyde nothandled unknown x,x
etryptamine nothandled unknown x,x
flavamine nothandled unknown x,x
```

```
fluoroformylone nothandled unknown x,x
fluoromethalone nothandled unknown x,x
fluorometholone nothandled unknown x,x
fluroxypyr nothandled unknown x,x
formamidoepoxide nothandled unknown x,x
formyldienolone nothandled unknown x,x
formylmethanofuran nothandled unknown x,x
fumarin nothandled unknown x,x
furalazine nothandled unknown x,x
furatoin nothandled unknown x,x
furfurin nothandled unknown x,x
gallamine nothandled unknown x,x
glucid nothandled unknown x,x
glyoxyldiureide nothandled unknown x,x
gonacrine nothandled unknown x,x
hexamethylenetetraamine nothandled unknown x,x
hexylthiocarbam nothandled unknown x,x
hydantal nothandled unknown x,x
hydantin nothandled unknown x,x
hydantoinal nothandled unknown x,x
hydantol nothandled unknown x,x
iodamide nothandled unknown x,x
iodixanol nothandled unknown x,x
iodoxamic nothandled unknown x,x
isopropalin nothandled unknown x,x
isopropamide root root CC([N+](CCC(C1=CC=CC=C1)(C2=CC=CC=C2)C(N)=O)(C(C)C)C)C,x
lactal nothandled unknown x,x
lactin nothandled unknown x,x
largon nothandled unknown x,x
laurenyne nothandled unknown x,x
laurine nothandled unknown x,x
lazo nothandled unknown x,x
lethane nothandled unknown x,x
leucol nothandled unknown x,x
lindane nothandled unknown x,x
lindol nothandled unknown x,x
lutidon nothandled unknown x,x
malonal nothandled unknown x,x
mesofolin nothandled unknown x,x
metachlorphenprop nothandled unknown x,x
methanopterin nothandled unknown x,x
methacetin nothandled unknown x,x
methacetone nothandled unknown x,x
methanofuran nothandled unknown x,x
metharsan nothandled unknown x,x
methazid nothandled unknown x,x
methazolamide root root CC(N=C1SC(S(N)(=O)=O)=NN1C)=O,x
methiodal nothandled unknown x,x
methionic nothandled unknown x,x
methoxychlor root root ClC(Cl)(Cl)C(C2=CC=C(OC)C=C2)C1=CC=C(OC)C=C1,x
methylaminopterin nothandled unknown x,x
methylenyl nothandled unknown x,x
methylone nothandled unknown x,x
monazan nothandled unknown x,x
monazol nothandled unknown x,x
monobenzone nothandled unknown x,x
montanine nothandled unknown x,x
```

```
morinamide nothandled unknown x,x
naphthonone nothandled unknown x,x
neonal nothandled unknown x,x
neophan nothandled unknown x,x
neraminol nothandled unknown x,x
nicetal nothandled unknown x,x
nicetamide nothandled unknown x,x
nitralin nothandled unknown x,x
nitrochlor nothandled unknown x,x
nitroglycerin nothandled unknown x,x
nitroglycerol nothandled unknown x,x
octatropine nothandled unknown x,x
ophthalamin nothandled unknown x,x
oxaine nothandled unknown x,x
oxamyl nothandled unknown x,x
oxanamide nothandled unknown x,x
oxanilide nothandled unknown x,x
oxanthrene nothandled unknown x,x
oxolamine root root CCN(CCC1=NC(C2=CC=CC=C2)=NO1)CC,x
oxophenarsine nothandled unknown x,x
oxoprostol nothandled unknown x,x
oxybutynin root root CCN(CC#CCOC(C(C1CCCCC1)(c2ccccc2)O)=O)CC,x
oxydiazol nothandled unknown x,x
oxyfume nothandled unknown x,x
oxylan nothandled unknown x,x
oxylite nothandled unknown x,x
pentalenene nothandled unknown x,x
pentalenolactone nothandled unknown x,x
pentanochlor nothandled unknown x,x
pernitr nothandled unknown x,x
persilic nothandled unknown x,x
phenactropinium nothandled unknown x,x
phenatine nothandled unknown x,x
phenatoine nothandled unknown x,x
phenazon nothandled unknown x,x
phenformin root root N=C(NC(N)=N)NCCC1=CC=CC=C1,x
phenonyl nothandled unknown x,x
phenoxethol nothandled unknown x,x
phenoxybenzamine nothandled unknown x,x
phenoxytol nothandled unknown x,x
phenvalerate nothandled unknown x,x
phloretin root root O=C(CCC2=CC=C(O)C=C2)C1=C(O)C=C(O)C=C1O,x
phosphaniline nothandled unknown x,x
phosphestrol nothandled unknown x,x
phosphotrienin nothandled unknown x,x
phthalazinol nothandled unknown x,x
phytin nothandled unknown x,x
pinacolin nothandled unknown x,x
piperazate nothandled unknown x,x
piperidolate root root O=C(OC2CN(CC)CCC2)C(C3=CC=CC=C3)C1=CC=CC=C1,x
pivalone nothandled unknown x,x
pivalyn nothandled unknown x,x
propal nothandled unknown x,x
propamidine nothandled unknown x,x
propargite nothandled unknown x,x
propazolamide nothandled unknown x,x
propiodal nothandled unknown x,x
```

```
propon nothandled unknown x,x
proponal nothandled unknown x,x
pyramin nothandled unknown x,x
pyrazofurin nothandled unknown x,x
pyrazolynate nothandled unknown x,x
pyrazon nothandled unknown x,x
pyridate nothandled unknown x,x
pyridazol nothandled unknown x,x
pyridenal nothandled unknown x,x
pyridene nothandled unknown x,x
pyrinamine nothandled unknown x,x
pyroxychlor nothandled unknown x,x
pyroxyfur nothandled unknown x,x
razide nothandled unknown x,x
razoxane nothandled unknown x,x
razoxane nothandled unknown x,x
razoxin nothandled unknown x,x
restran nothandled unknown x,x
restryl nothandled unknown x,x
roxindole nothandled unknown x,x
roxion nothandled unknown x,x
saccharimide nothandled unknown x,x
serinal nothandled unknown x,x
shoxin nothandled unknown x,x
silantin nothandled unknown x,x
soxinol nothandled unknown x,x
stoxil nothandled unknown x,x
styron nothandled unknown x,x
sulfacid nothandled unknown x,x
sulfalene nothandled unknown x,x
sulfamethazine|sulfamethazin nothandled unknown x,x
sulfamethin nothandled unknown x,x
sulfodiazol nothandled unknown x,x
sulfurine nothandled unknown x,x
sulfurol nothandled unknown x,x
syncurine nothandled unknown x,x
synhexyl nothandled unknown x,x
synoestron nothandled unknown x,x
synpren nothandled unknown x,x
syringin nothandled unknown x,x
talon nothandled unknown x,x
tartran nothandled unknown x,x
terbolan nothandled unknown x,x
terbut nothandled unknown x,x
terbutaline nothandled unknown x,x
terbutol nothandled unknown x,x
teroxalene nothandled unknown x,x
tetralide nothandled unknown x,x
tetralite nothandled unknown x,x
tetrathiin nothandled unknown x,x
thenylchlor nothandled unknown x,x
thenylene nothandled unknown x,x
thenylpyramine nothandled unknown x,x
thiabenzazole nothandled unknown x,x
thiabenzazonium nothandled unknown x,x
thiadiazinol nothandled unknown x,x
thiamylal root root S=C(N1)NC(C(C(C)CCC)(CC=C)C1=O)=O,x
```

```
thiazopyr nothandled unknown x,x
thioallate nothandled unknown x,x
thiocuran nothandled unknown x,x
thionylan nothandled unknown x,x
thioxamyl nothandled unknown x,x
thorazine nothandled unknown x,x
tolamide nothandled unknown x,x
tolamine nothandled unknown x,x
tolbutamide root root O=C(NS(C1=CC=C(C)C=C1)(=O)=O)NCCCC,x
tolcyclamide nothandled unknown x,x
tolite nothandled unknown x,x
tolnaphthate nothandled unknown x,x
tolpentamide nothandled unknown x,x
tolpropamine nothandled unknown x,x
transamine nothandled unknown x,x
triazbutyl nothandled unknown x,x
triazinate nothandled unknown x,x
tricinolon nothandled unknown x,x
tricuran nothandled unknown x,x
tropium nothandled unknown x,x
uridinal nothandled unknown x,x
ustilan nothandled unknown x,x
uval nothandled unknown x,x
uvon nothandled unknown x,x
vanillone nothandled unknown x,x
vinformide nothandled unknown x,x
vulvan nothandled unknown x,x
xanthinol nothandled unknown x,x
zded nothandled unknown x,x
zolamine nothandled unknown x,x
zoxazolamine root root NC2=NC1=CC(Cl)=CC=C1O2,x
trans unknown unknown x,x
alltrans unknown unknown x,x
cis unknown unknown x,x
allcis unknown unknown x,x
syn|anti unknown unknown x,x
endo unknown unknown x,x
high unknown unknown x,x
analysis|analytical unknown unknown x,x
aqueous|nonaqueous unknown unknown x,x
laser unknown unknown x,x
phosphoruspentoxide unknown unknown x,x
%|moll|mgml|microgml|glt|mesh|mm|cm|ml|ppm|micron|microns stopword percent x,x
0m|1m|2m|3m|4m|5m|6m|7m|8m|9m|0n|1n|2n|3n|4n|5n|6n|7n|8n|9n stopword percent x,x
ing|ed stopword ing x,x
grade|purity|solution|standardsolution stopword grade x,x
7ci|8ci|9ci|10ci stopword toend x,x
aas|absolute|acn|acs|acsreagent|activator|aerosol|amorphous|analytical stopword
toend x,x
analyzer|anhydrous|approx|assay|atomic stopword toend x,x
balance|beads|bifunctional|biochemical|briquette|briquettes stopword toend x,x
capacity|chelometric|chemiluminescence|certified|chip|chips stopword toend x,x
chiral|chunk|chunks|coarse|colloidal|colorless|concentrate|contains stopword
toend x,x
crucible|crucibles|crude|crystal|crystallites|crystals|crystalline|cube stopword
toend x,x
denatured|determination|dispersion|dry|dust stopword toend x,x
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each|electrolytic|electronic|electrophoresis|environmental|esterification|extrac
tion|extrapure stopword toend x,x
fcc|filings|fine|finest|flake|flakes|fluorescent|fluorimetric|foil|for|freeradic
al|from|fume stopword toend x,x
gas|gauze|gcstandard|glacial|granular|granulate|granule|granules stopword toend
x,x
heavy|hplc|hydrophobic stopword toend x,x
indicator|ingot|ingots|iupac stopword toend x,x
light|liquid|loose|low|lump|lumps stopword toend x,x
mainly|maycontain|metal|metals|minimum|moist|mossy stopword toend x,x
native|natural|needle|needles|notstabilized stopword toend x,x
on|onactivatedcarbon|optical|organic stopword toend x,x
particle|pearl|pearls|pellet|pellets|photopolymerization|piece|pieces|plasticize
r stopword toend x,x
plate|plates|porous|powder|pract|practical|predominantly|predominatly|primarysta
ndard|puratronic|pure|purum stopword toend x,x
reagent|reagentfor|reagentacs|redox|reference|remainder|research|ribbon|ribbons|
rod|rods stopword toend x,x
scale|scales|scoop|secondarystandard|selective|sensitive|shaving|shavings|shot
stopword toend x,x
simultaneous|singlecrystal|slug|slugs|soft|solid|solution|soot|spectrographic|sp
ectrophotometric stopword toend x,x
sphere|spheres|spin|sponge|spray|stab|stabilized|stable|standard|stick|sticks|su
spension|synthetic|syrup|syrupy stopword toend x,x
tablet|tablets|tech|technical|thinfoil|titrant|topical|turnings|typically
stopword toend x,x
ultra|ultrapure|unstabilized|ultrathinfoil|usp|uvgrade stopword toend x,x
vial|volumetricstandard stopword toend x,x
wet|wire|wires|wool stopword toend x,x
zonerefined stopword toend x,x
24d|245t|24dnp buildable unknown x,x
thinfoil|ultrathinfoil|singlecrystal buildable unknown x,x
antibovine|anticat|antichicken|antidog|antigoat|antiguineapig|antihorse|antihuma
n|antimonkey|antirabbit|antirat|antisheep notthisversion macromolecule x,x
tetrahydroprogesterone|tetrahydroprogesteron buildable unknown x,x
hydrofluoride|hydrochloride|methochloride|methobromide|hydrobromide|hydroiodide|
hydriodide|methoiodide|methiodide|ethoiodide|ethiodide buildable unknown x,x
cyclopentadefphenanthren|cyclopentadefphenanthrene buildable unknown x,x
1011dihydrocinchon|1011dihydrocinchonine|1011dihydrocinchonin|1011dihydroquinidi
ne|1011dihydrocinchonidine|1011dihydrocinchonidin buildable unknown x,x
1011dihydroquinine|1011dihydroquinin|dihydroquinine|dihydroquinin|hydroquinine|h
ydroquinin buildable unknown x,x
alphaergocryptine|alphaergocryptin|alphaergocriptine|alphaergocriptin buildable
unknown x,x
betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|
bergocryptin|bergocriptine|bergocriptin buildable unknown x,x
alphaergocryptinine|alphaergocryptinin|alphaergocriptinine|alphaergocriptinin
buildable unknown x,x
betaergocryptinine|betaergocryptinin|betaergocriptinine|betaergocriptinin|bergoc
ryptinine|bergocryptinin|bergocriptinine|bergocriptinin buildable unknown x,x
1alphah5alphahtropan buildable unknown x,x
ethylvanillin|ethylcitral buildable unknown x,x
orthocatechol buildable unknown x,x
isatoicanhydride buildable unknown x,x
cresylicacid buildable unknown x,x
chlorosulfamicacid buildable unknown x,x

100

hexafluorophosphoricacid|hexafluorosilicicacid|hexafluorozirconicicacid|tetraflu
oroboricacid buildable unknown x,x
ylcation|ylanion buildable unknown x,x
betaalan buildable unknown x,x
crotonylalcohol buildable unknown x,x
betainealdehyde|betainaldehyd buildable unknown x,x
biotinamide|biotinamid buildable unknown x,x
angeldust buildable unknown x,x
catecholborane buildable unknown x,x
vitaminb1nitrate|thiaminenitrate|thiaminnitrate|thiaminechloride|thiaminchlorid
buildable unknown x,x
44'carbocyanine|22'carbocyanine buildable unknown x,x
ylthiol buildable unknown x,x
benzeneoxid|benzeneoxide buildable unknown x,x
card|2022cardenolide|card2022enolide buildable unknown x,x
25norbornadien|25norbornadiene|2norbornene|2norbornen|5norbornene|5norbornen
buildable unknown x,x
icalcohol buildable unknown x,x
orthophthal buildable unknown x,x
neopentylglycol buildable unknown x,x
nitrogendioxide|nitricoxide|nitrousoxide buildable unknown x,x
hydrogenphosphato|dihydrogenphosphato buildable unknown x,x
chloralhydrate|bromalhydrate buildable unknown x,x
vinylsulfurol buildable unknown x,x
arsenicacid buildable unknown x,x
methacr buildable unknown x,x
formamidinedisulfide buildable unknown x,x
isonitroso|isonitros|isonipecot|isobenzofuran|isocrotono|isocroton|isocrot|isoqu
inol|isochinol|glutathionereduced buildable unknown x,x
3thiotriphosphor|2thiodiphosphor buildable unknown x,x
alphalinolen|gammalinolen buildable unknown x,x
alphaglycerophosph|1alphaglycerophosph|dalphaglycerophosph|dlalphaglycerophosph
buildable unknown x,x
alphaglycerophospho|1alphaglycerophospho|dalphaglycerophospho|dlalphaglycerophos
pho buildable unknown x,x
betaoestradiol|betaestradiol buildable unknown x,x
dicarboxylicimide|dicarboxylicacidimide buildable unknown x,x
hydrogentartrate|hydrogenltartrate|hydrogendtartrate|lbitartrate|dbitartrate|hyd
rogenmaleate|hydrogenoxalate|hydrogensulfate|hydrogensulfite|hydrogensulfide
buildable unknown x,x
alphaionon|alphaionone|betaionone|betaionon buildable unknown x,x
sulfurdiimide|sulfurdiimid buildable unknown x,x
snglycerol|snglycero|racglycerol|racglycero buildable unknown x,x
orthophosphor buildable unknown x,x
uvgrade buildable unknown x,x
ionchromatography buildable unknown x,x
dewarbenzene buildable unknown x,x
alloisoleuc|allothreono|allothreon buildable unknown x,x
anaphthoflavone|alphanaphthoflavone|bnaphthoflavone|betanaphthoflavone buildable
unknown x,x
gcstandard|primarystandard|secondarystandard buildable unknown x,x
purineriboside buildable unknown x,x
secpheneth buildable unknown x,x
4nitroanilide|pnitroanilide buildable unknown x,x
betacitronell buildable unknown x,x
methylviologen|ethylviologen|benzylviologen buildable unknown x,x
zirconyliv|vanadyliv buildable unknown x,x

activatedcarbon|onactivatedcarbon buildable unknown x,x
extrapure buildable unknown x,x
maycontain buildable unknown x,x
volumetricstandard buildable unknown x,x
notstabilized buildable unknown x,x
zonerefined buildable unknown x,x
standardsolution buildable unknown x,x
wt buildable unknown x,x
phosphorustriamide buildable unknown x,x
nepsilon buildable unknown x,x
betacarboline buildable unknown x,x
pentamethylenetetramine|pentamethylenetetramin buildable unknown x,x
hexamethylenetetramine|hexamethylenetetramin buildable unknown x,x
ochloranil|mchloranil|pchloranil buildable unknown x,x
mesoinositol|myoinositol|dinositol|linositol|scylloinositol|epiinositol
buildable unknown x,x
stainlesssteel buildable unknown x,x
alphafuril buildable unknown x,x
alphapinene|betapinene buildable unknown x,x
chrysoidiner buildable unknown x,x
naphtholas buildable unknown x,x
neutralbuffer buildable unknown x,x
alphacumyl buildable unknown x,x
alphaphellandrene|betaphellandrene buildable unknown x,x
bisphenola buildable unknown x,x
alphalip|alip buildable unknown x,x
alpharesorcyl|aresorcyl|betaresorcyl|bresorcyl|gammaresorcyl|gresorcyl buildable
unknown x,x
gerani buildable unknown x,x
lascorb buildable unknown x,x
vitaminh|vitaminb1|thiaminedisulfide|vitaminb2|vitamine|alphatocopherol|atocophe
rol buildable unknown x,x
vitamind3 buildable unknown x,x
phenolsulfonphthalein|phenolsulfonephthalein|mcresolsulfonphthalein|mcresolsulfo
nephthalein|ocresolsulfonphthalein|ocresolsulfonephthalein|pyrocatecholsulfonpht
halein|pyrocatecholsulfonephthalein|pyrogallolsulfonphthalein|pyrogallolsulfonep
hthalein|thymolsulfonphthalein|thymolsulfonephthalein|phenolphthalein|mcresolpht
halein|ocresolphthalein|pyrocatecholphthalein|pyrogallolphthalein|thymolphthalei
n buildable unknown x,x
freeradical buildable unknown x,x
obenzeno buildable unknown x,x
ptoluquinone|pxyloquinone buildable unknown x,x
cyclopentaaphenanthrene|cyclopentaaphenanthren buildable unknown x,x
pdioxine|mdioxine|pdioxin|mdioxin buildable unknown x,x
asindacene|asindacen|sindacene|sindacen buildable unknown x,x
sendachromeal buildable unknown x,x
isonicotino|isonicotin buildable unknown x,x
leucicacid buildable unknown x,x
isoser buildable unknown x,x
isoval buildable unknown x,x
isoleuc buildable unknown x,x
tleuc|tertleuc buildable unknown x,x
orthotyros buildable unknown x,x
mtyros|metatyros buildable unknown x,x
ptyros|paratyros buildable unknown x,x
hydroxyprol|3hydroxyprol|4hydroxyprol|5hydroxyprol buildable unknown x,x
3phenylalan|betaphenylalan buildable unknown x,x

```
dtartar|dtartr|mesotartar|mesotartr buildable unknown x,x
tetrafluoroborate|tetrafluoroborate1 buildable unknown x,x
fluorosilicate|fluorosilicat|hexafluorosilicate|hexafluorosilicat buildable
unknown x,x
onnazoxy|nnoazoxy|nonazoxy buildable unknown x,x
glycolacetal|glycolketal buildable unknown x,x
moll|mgml|microgml|glt|reagentfor|reagentacs|acsreagent buildable unknown x,x
ptosylate|ptosyl buildable unknown x,x
oxazine1|oxazine4 buildable unknown x,x
tboc buildable unknown x,x
iumion|ideion|iumcation|ideanion buildable unknown x,x
isobutyro|isobutyr buildable unknown x,x
isovalero|isovaler buildable unknown x,x
isophthalo|mphthalo|isophthal|mphthal buildable unknown x,x
terephthalo|pphthalo|terephthal|pphthal buildable unknown x,x
etherof buildable unknown x,x
esterswith|estersof|esterwith|esterof buildable unknown x,x
saltof buildable unknown x,x
iclactone|iclacton buildable unknown x,x
iclactam buildable unknown x,x
anhydridewith buildable unknown x,x
cyclicanhydride buildable unknown x,x
phosphoruspentoxide buildable unknown x,x
allcis buildable unknown x,x
alltrans buildable unknown x,x
acinitro buildable unknown x,x
astriazine|astriazin|striazine|striazin|asymtriazine|asymtriazin|symtriazine|sym
triazin buildable unknown x,x
astrioxane|astrioxan|strioxane|strioxan|asymtrioxane|asymtrioxan|symtrioxane|sym
trioxan buildable unknown x,x
astriazino|striazino|asymtriazino|symtriazino buildable unknown x,x
astrioxano|strioxano|asymtrioxano|symtrioxano buildable unknown x,x
astrithiane|astrithian|strithiane|strithian|asymtrithiane|asymtrithian|symtrithi
ane|symtrithian buildable unknown x,x
thiurammonosulfide|thiuramdisulfide|thiuramtrisulfide|thiuramtrisulfid|thiuramte
trasulfide|thiuramtetrasulfid buildable unknown x,x
isourea|isothiourea|1isoureido|3isoureido|1isothioureido|3isothioureido|1isosele
noureido|3isoselenoureido|1isotelluroureido|3isotelluroureido buildable unknown
x,x
` typo typo '
" typo typo ''
± typo typo +/-
µ typo typo mu
,- typo typo -
§ typo typo beta
-> typo typo -fwdarw-
(alpha) typo typo alpha
(beta) typo typo beta
(gamma) typo typo gamma
(delta) typo typo delta
(epsilon) typo typo epsilon
(omega) typo typo omega
(ortho) typo typo ortho
(meta) typo typo meta
(para) typo typo para
(tau) typo typo tau
-oxyl typo typo -oxylradical
```

```
-thiolate typo typo -mercaptide
1-dimethylaminonaphthalene-5-sulfonyl typo typo dansyl
1,2-o-isopropylidene-d-glycer typo typo 2,3-o-isopropylidene-d-glycer
1,2-o-isopropylidene-l-glycer typo typo 2,3-o-isopropylidene-l-glycer
1,2-o-isopropylidene-glycer typo typo 2,3-o-isopropylidene-glycer
1alphah,5alphah typo typo 1alphah5alphah
a.c.s typo typo acs
acetonamin typo typo acetonylamin
acxid typo typo acid
adonitol typo typo ribitol
aicd typo typo acid
aldazine typo typo aldehydeazine
all-e typo typo all-cis
all-z typo typo all-trans
allose typo typo alloose
allofuranose typo typo alloofuranose
allopyranose typo typo alloopyranose
alpha-tolual typo typo phenylacetal
alpha-toluat typo typo phenylacetat
alpha-toluic typo typo phenylacetic
alpha-tolunitril typo typo phenylacetonitril
aluminium typo typo aluminum
amidosulfon typo typo amidosulfur
amimo typo typo amino
ammin typo typo amin
anonan typo typo a-nonan
anonyl typo typo a-nonyl
azodicarbonamide typo typo azodicarboxamide
bathophenanthroline typo typo bathophenanthroline
benez typo typo benz
benzamin typo typo benzenamin
benzhydrazid typo typo benz-hydrazid
benzhydroxam typo typo benz-hydroxam
benzotriazoyl typo typo benzotriazolyl
bisoleam typo typo bis-oleam
bismeth typo typo dimeth
borinan typo typo bor-inan
caes typo typo ces
capro typo typo hexano
caprin typo typo decan
carboselen typo typo carboxselen
carbotellur typo typo carboxtellur
carbothi typo typo carboxthi
carboxamide typo typo carboxylamide
chinone typo typo quinone
chlorobromide typo typo chloridebromide
chlorofluoride typo typo chloridefluoride
chloroformate typo typo (chloroformate)
cinnamid typo typo cinnamamid
cis/trans typo typo cis+trans
collidin typo typo trimethylpyridin
columb typo typo niob
crotonitrile typo typo crotononitrile
dextrose typo typo d-glucose
dicaprin typo typo dicapr-in
diethylenetriaminepenta typo typo diethylenetriamine-n,n,n',n',n''-penta
diethylenetriamine-penta typo typo diethylenetriamine-n,n,n',n',n''-penta
```

dioleate typo typo di-oleate
dioleoyl typo typo di-oleoyl
dionate typo typo -dionate
diphosphate typo typo diphosphorate
ehty typo typo ethy
endo, typo typo endo-
erythrul typo typo glycerotetrul
ethinyl typo typo ethynyl
ethylenebis typo typo ethylene-bis-
ethylenediaminetetra typo typo ethylenediamine-n,n,n',n'-tetra
ethylhexoxid typo typo ethylhexanoxid
etyhl typo typo ethyl
exo, typo typo exo-
flour typo typo fluor
fluoronon typo typo fluoro-non
fluro typo typo fluoro
furanuron typo typo furanoseuron
fruct typo typo arabinohexul
fucosyl typo typo fucoseyl
galactosyl typo typo galactoseyl
gamma-collidin typo typo 2,4,6-trimethylpyridin
glucosyl typo typo glucoseyl
glucuronide typo typo glucosiduronicacid
guanad typo typo guanid
hydrofluoren typo typo hydro-fluoren
idose typo typo idoose
idofuranose typo typo idoofuranose
idopyranose typo typo idoopyranose
imadaz typo typo imidaz
imdaz typo typo imidaz
inosinate typo typo inosate
inosinic typo typo inosic
iso- typo typo iso
levulo typo typo arabinohexulo
linalyl typo typo linaloyl
lupetid typo typo dimethylpiperid
lutid typo typo dimethylpyrid
mol/l typo typo moll
monocaprin typo typo monocapr-in
mononitrile typo typo mono-nitrile
monoole typo typo mono-ole
mucic typo typo galactaric
n'n' typo typo n',n'
n-alpha typo typo nalpha
n-(alpha) typo typo nalpha
n-gamma typo typo ngamma
n-delta typo typo ndelta
n-omega typo typo nomega
n-im- typo typo nim
naphta typo typo naphtha
naphthaldehyde typo typo naphthaldehyde
naphthalic typo typo naphthalenedicarboxylic
naphthalimid typo typo naphthalenedicarboximid
naphty typo typo naphthy
naphthyrid typo typo diazanaphthalene
napta typo typo naphtha
napth typo typo naphth

```
napty typo typo naphthy
ocineol typo typo o-cineol
oxamide typo typo oxalicamide
oxeturon typo typo oxetoseuron
oxiruron typo typo oxiroseuron
oxylenol typo typo o-xylenol
p-naphthoquinone typo typo 1,4-naphthoquinone
pentacyclohexylammonium typo typo penta(cyclohexylammonium)
peracet typo typo peroxyacet
phath typo typo phth
phenanthroline typo typo diazabenzo[a]naphthalene
phosphonyl typo typo phosphonoyl
phosphorin typo typo -phosphorin
phosphoryl typo typo phosphoroyl
phtal typo typo phthal
phthaldehyde typo typo phthalaldehyde
proprion typo typo propion
pthal typo typo phthal
psico typo typo ribohexulo
pyranuron typo typo pyranoseuron
rhodate typo typo rhodaate
ribul typo typo erythropentul
rosinate typo typo abietate
s-triazol typo typo 1,2,4-triazol
sacchar typo typo glucar
saccharin typo typo saccharin
saccharid typo typo saccharid
salycyl typo typo salicyl
selenious typo typo selenous
septanuron typo typo septanuron
siloxid typo typo silanoxid
sorbo typo typo xylohexulo
sorbitol typo typo glucitol
stilbazol typo typo styrylpyridin
sufo typo typo sulfo
sulfamidic typo typo sulfamic
sulfamyl typo typo sulfamoyl
sulfohydrazide typo typo sulfonohydrazide
sulph typo typo sulf
sulphamyl typo typo sulfamoyl
sulphohydrazide typo typo sulfonohydrazide
tagat typo typo lyxohexul
tetracarboxdiimide typo typo bis(dicarboximide)
tetrahydridoborato typo typo tetrahydridoborate
tetraphosphate typo typo tetraphosphorate
thiazyl typo typo thiazolyl
thiocarbamyl typo typo thiocarbamoyl
thiol- typo typo thiole-
thiolan typo typo thi-olan
thiolylium typo typo thiole-ylium
thionochloroform typo typo chlorothionoform
thiooxine typo typo thio(oxine)
thiophen- typo typo thiophene-
thiophenamine typo typo thiophene-amine
thiophenic typo typo thiopheneic
thiophenone typo typo thiophene-one
threonate typo typo threoonate
```

```
threonic typo typo threoonic
tricaprin typo typo tricapr-in
tricaproin typo typo trihexanoin
trichloromethylsulfen|trichloromethanesulfen typo typo (trichloromethyl)sulfen
trifluoromethylsulfen|trifluoromethanesulfen typo typo (trifluoromethyl)sulfen
trioleate typo typo (tris)oleate
triolein typo typo tri-ole-in
trioleoyl typo typo (tris)oleoyl
trioleyl typo typo (tris)oleyl
triphosphate typo typo triphosphorate
trithioperoxy typo typo thiodithioperoxy
tritolyl typo typo tristolyl
tropilidene typo typo 2,4,6-cyclohexatriene
tyrosinate typo typo tyrosin-ate
uloson typo typo ulo-on
xanthylic typo typo xanthonylic
xylul typo typo threopentul
acidic notthisversion unknown x,x
activatedcarbon notthisversion bulksolid x,x
agarose notthisversion macromolecule x,x
agar notthisversion macromolecule x,x
agglutinin notthisversion macromolecule x,x
albumin notthisversion macromolecule x,x
alkonium notthisversion mixture x,x
alkyl|alkyl* notthisversion mixture x,x
alloy notthisversion bulksolid x,x
algin notthisversion macromolecule x,x
alumina notthisversion bulksolid x,x
amalgam notthisversion bulksolid x,x
amyloid notthisversion macromolecule x,x
amylose notthisversion macromolecule x,x
angiotensin notthisversion macromolecule x,x
anthocyanidin notthisversion mixture x,x
anthocyanin notthisversion mixture x,x
antibody notthisversion macromolecule x,x
antibovine notthisversion macromolecule x,x
anticat notthisversion macromolecule x,x
antichicken notthisversion macromolecule x,x
antidog notthisversion macromolecule x,x
antigoat notthisversion macromolecule x,x
antiguineapig notthisversion macromolecule x,x
antihorse notthisversion macromolecule x,x
antihuman notthisversion macromolecule x,x
antimonkey notthisversion macromolecule x,x
antirabbit notthisversion macromolecule x,x
antirat notthisversion macromolecule x,x
antisheep notthisversion macromolecule x,x
ase notthisversion macromolecule x,x
asphalt notthisversion mixture x,x
avidin notthisversion macromolecule x,x
azure notthisversion color x,x
bacitracin notthisversion macromolecule x,x
bead|beads notthisversion bulksolid x,x
bentonite notthisversion bulksolid x,x
black notthisversion color x,x
block notthisversion polymer x,x
blue notthisversion color x,x
```

bombesin notthisversion macromolecule x,x
bradykinin notthisversion macromolecule x,x
brij notthisversion polymer x,x
brilliant notthisversion color x,x
bromelian notthisversion macromolecule x,x
broth notthisversion mixture x,x
brown notthisversion color x,x
buckyball|buckyballs notthisversion fullerene x,x
buffer notthisversion mixture x,x
calcia notthisversion bulksolid x,x
calcitonin notthisversion macromolecule x,x
carborundum notthisversion bulksolid x,x
carmine notthisversion color x,x
carrageenan notthisversion macromolecule x,x
casein notthisversion macromolecule x,x
casomorphin notthisversion macromolecule x,x
celite notthisversion bulksolid x,x
cells notthisversion bulksolid x,x
cellulose notthisversion macromolecule x,x
cephalin|cephalins notthisversion mixture x,x
ceria notthisversion bulksolid x,x
charcoal notthisversion bulksolid x,x
chelate notthisversion mixture x,x
chitin notthisversion macromolecule x,x
chitosan notthisversion macromolecule x,x
cholecystokinin notthisversion macromolecule x,x
chondroitin notthisversion macromolecule x,x
cocktail notthisversion mixture x,x
coco notthisversion mixture x,x
collagen notthisversion macromolecule x,x
collodion notthisversion macromolecule x,x
concanavalin notthisversion macromolecule x,x
conotoxin notthisversion macromolecule x,x
demi notthisversion hemi x,x
detergent|detergent notthisversion mixture x,x
dextrin|dextran notthisversion macromolecule x,x
dna notthisversion macromolecule x,x
dowex notthisversion polymer x,x
drierite notthisversion bulksolid x,x
dynorphin notthisversion macromolecule x,x
edestin notthisversion macromolecule x,x
endorphin notthisversion macromolecule x,x
endothelin notthisversion macromolecule x,x
enzyme|enzymes notthisversion macromolecule x,x
emulsin notthisversion macromolecule x,x
extract notthisversion mixture x,x
fatty notthisversion mixture x,x
ferritin notthisversion macromolecule x,x
fibrin notthisversion macromolecule x,x
fibrinogen notthisversion macromolecule x,x
fibrinolysin notthisversion macromolecule x,x
fibronectin notthisversion macromolecule x,x
ficin notthisversion macromolecule x,x
ferrocene|ferrocen notthisversion inorgcomplex x,x
flavor notthisversion mixture x,x
fraction notthisversion mixture x,x
fullerene|fullerenes notthisversion fullerene x,x

```
galactan notthisversion polymer x,x
gelatin|gelatine notthisversion macromolecule x,x
gliadin notthisversion macromolecule x,x
globulin notthisversion macromolecule x,x
glove|gloves notthisversion bulksolid x,x
gluten notthisversion macromolecule x,x
glutenin notthisversion macromolecule x,x
gonadotropin notthisversion macromolecule x,x
graphite notthisversion bulksolid x,x
green notthisversion color x,x
grey|gray notthisversion color x,x
gum notthisversion mixture x,x
hemi notthisversion hemi x,x
hemoglobin notthisversion macromolecule x,x
heparin|heparan notthisversion macromolecule x,x
histone notthisversion macromolecule x,x
hormone notthisversion macromolecule x,x
hyaluron notthisversion macromolecule x,x
hydrocarbon|hydrocarbons notthisversion mixture x,x
insulin notthisversion macromolecule x,x
interferon notthisversion macromolecule x,x
interleukin notthisversion macromolecule x,x
inulin notthisversion macromolecule x,x
isotope notthisversion isotope x,x
kaolin notthisversion macromolecule x,x
kephalin notthisversion macromolecule x,x
keratin notthisversion macromolecule x,x
kerosene|kerosine notthisversion mixture x,x
kit notthisversion mixture x,x
kitasamycin notthisversion mixture x,x
lake notthisversion color x,x
laminaran notthisversion macromolecule x,x
lanolin notthisversion macromolecule x,x
latex notthisversion polymer x,x
lecithin notthisversion macromolecule x,x
lectin notthisversion macromolecule x,x
lignine|lignin notthisversion macromolecule x,x
ligroin|ligroine notthisversion mixture x,x
litmus notthisversion macromolecule x,x
lysozyme notthisversion macromolecule x,x
magenta notthisversion color x,x
mannan notthisversion macromolecule x,x
mixed|mixt|mixture|mixtures notthisversion mixture x,x
mer|mers notthisversion polymer x,x
merase notthisversion macromolecule x,x
mu notthisversion inorgcomplex x,x
mucin notthisversion macromolecule x,x
myoglobin notthisversion macromolecule x,x
myosin notthisversion macromolecule x,x
naphthen notthisversion macromolecule x,x
neurokinin notthisversion macromolecule x,x
neurotensin notthisversion macromolecule x,x
nigrosine notthisversion macromolecule x,x
norit notthisversion bulksolid x,x
nucle notthisversion macromolecule x,x
nuclein notthisversion macromolecule x,x
nylon notthisversion polymer x,x
```

```
ocene|ocen notthisversion inorgcomplex x,x
oil notthisversion mixture x,x
orange notthisversion color x,x
pancreatin notthisversion macromolecule x,x
papain notthisversion macromolecule x,x
paraffin notthisversion bulksolid x,x
paraformaldehyde notthisversion polymer x,x
parathyroid notthisversion macromolecule x,x
pectin notthisversion macromolecule x,x
pepsin notthisversion macromolecule x,x
peptide notthisversion macromolecule x,x
peptone notthisversion macromolecule x,x
petrol|petroleum notthisversion mixture x,x
pink notthisversion color x,x
pipe notthisversion bulksolid x,x
pollen notthisversion bulksolid x,x
poly|polymer|polymers|homopolymer notthisversion polymer x,x
protamine notthisversion macromolecule x,x
protein notthisversion macromolecule x,x
pullulan notthisversion macromolecule x,x
purple notthisversion color x,x
quinhydrone notthisversion mixture x,x
red notthisversion color x,x
rennin notthisversion macromolecule x,x
resin notthisversion polymer x,x
rna notthisversion macromolecule x,x
salmine notthisversion macromolecule x,x
sand notthisversion bulksolid x,x
saponin notthisversion macromolecule x,x
scarlet notthisversion color x,x
semi notthisversion hemi x,x
serum notthisversion macromolecule x,x
sesqui notthisversion hemi x,x
sieve|sieves notthisversion bulksolid x,x
silica|silicagel notthisversion bulksolid x,x
somatostatin notthisversion macromolecule x,x
somatotropin notthisversion macromolecule x,x
stainlesssteel notthisversion bulksolid x,x
starch notthisversion macromolecule x,x
streptavidin notthisversion macromolecule x,x
streptomycin notthisversion macromolecule x,x
strip|strips notthisversion bulksolid x,x
talc notthisversion bulksolid x,x
tallow notthisversion mixture x,x
tann notthisversion macromolecule x,x
thaumatin notthisversion macromolecule x,x
thoria notthisversion bulksolid x,x
thrombin notthisversion macromolecule x,x
titania notthisversion bulksolid x,x
tragacanth notthisversion macromolecule x,x
transferrin notthisversion macromolecule x,x
triton notthisversion polymer x,x
trypsin notthisversion macromolecule x,x
tube|tubes notthisversion bulksolid x,x
tween notthisversion polymer x,x
tylose notthisversion macromolecule x,x
valve notthisversion bulksolid x,x
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vasopressin notthisversion macromolecule x,x
venom notthisversion mixture x,x
violet notthisversion color x,x
wax notthisversion bulksolid x,x
white notthisversion color x,x
xylan notthisversion macromolecule x,x
yeast notthisversion bulksolid x,x
yellow notthisversion color x,x
yttria notthisversion bulksolid x,x
zein notthisversion macromolecule x,x
zeolite notthisversion bulksolid x,x
zephiran notthisversion macromolecule x,x
zephirol notthisversion macromolecule x,x
zirconia notthisversion bulksolid x,x
zyme notthisversion macromolecule x,x
ortho ordinal ordinal x,x
epsilon ordinal ordinal x,x
nepsilon ordinal ordinal x,x
npi ordinal ordinal x,x